MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Materials' Revolution: Computational Design and Discovery of Novel Materials

Progress Report

Year 5

February 2018 - January 2019

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

Les Pôles de recherche nationaux (PRN) sont un instrument d'encouragement du Fonds national suisse
Die Nationalen Forschungsschwerpunkte (NFS) sind ein Förderungsinstrument des Schweizerischen Nationalfonds
I Poli di ricerca nazionali (PRN) sono un mezzo di sostegno del Fondo Nazionale Svizzero
The National Centres of Competence in Research (NCCR) are a research instrument of the Swiss National Science Foundation

Contents

1 Major developments in year 5

1.1 Research

Year 5 sees six design-and-discovery and two incubators projects fully operational, in addition to the Open Science and HPC and Future Architectures platforms. We report below the research status and milestones for each of these.

D&D1 — Understanding complex molecular crystals: structure and properties

Project leader: Michele Ceriotti (EPFL, 1MC)
Computational partners: Clémence Corminboeuf (EPFL, 2MC), **Stefan Goedecker** (UniBas, 1.5MC), **Michele Parrinello** (USI and ETHZ, 1.5MC), Anatole von Lilienfeld (UniBas)
Experimental partners: Esther Amstad (EPFL), Lyndon Emsley (EPFL)

Status of the project

The six sub-projects have been moving forward very fast, also thanks to the preparatory work laid out in phase I: (a) Accurate energetics and properties for molecular crystals; (b) Molecular and crystal energetics by machine learning (ML); (c) Anharmonic and quantum free energies; (d) Predicting complex properties by machine learning; (e) Molecular conformers and crystal structure search; (f) Interface energies and nucleation kinetics.

The computational partners have made progress on several fronts. A library of high-end reference calculations for prototypical molecular materials (**O**rg**A**nic **S**em**I**conductor**S**: OASIS database) has been expanding, and currently contains 14 fairly large compounds [a] [1]. A collective variable based on an approximate measure of configurational entropy [2] has been extended to include orientational correlations, which made it possible to explore polymorphism of molecular materials, including the discovery of entropy-stabilized phases [f] [3]. The release of the version 2.0 of the i-PI software [4] provides the infrastructure to implement advanced free-energy methods to estimate quantum and anharmonic free energies [c] [39, 40].

Furthermore, collaborative efforts have been established and are already making progress. A collaboration between the Goedecker, Corminboeuf, Ceriotti, and von Lilienfeld groups is surveying approaches to generate a forcefield for bare and capped aminoacids, using both local optimized conformers [41][5], and distorted configurations obtained from a minima hopping run [a,b,e]. Remarkable results have been obtained from the point of view of obtaining accurate ML predictions for experimentally measurable properties that are relevant for the characterization of molecular solids [d].

A collaboration between the Ceriotti and the Emsley group resulted in the ShiftML model, based on SOAP kernels, Gaussian process regression, and GIPAW-DFT reference calculations, that can predict nuclear chemical shieldings with an accuracy that is sufficient for NMR crystallography [6]. A web-based version has been made available on Materials Cloud (directly accessible through shiftml.org), and further extensions to more chemically complex compounds, and to out-of-equilibrium geometries, are currently being worked on. A collaboration between the Ceriotti and Corminboeuf groups has also developed a sophisticated scheme to machine-learn the electronic charge density, that could be used to improve X-ray crystallography, to accelerate density-functional calculations [7], and to compute density-based indicators of chemical

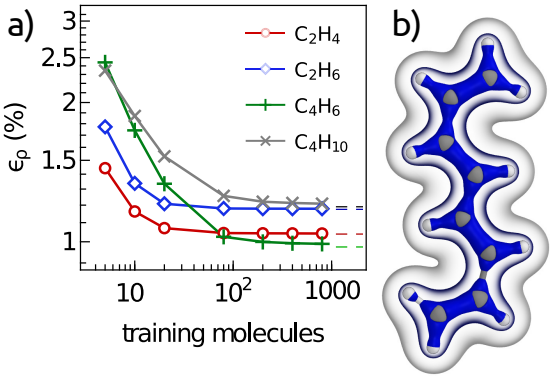

Figure 1: *A symmetry-adapted model of the electron density (a) reaches rapidly the accuracy set by the basis set expansion, when trained on small molecules, and (b) can be transferred to make predictions on larger, more complex compounds.*

bonding [8]. By using a symmetry-adapted machine-learning scheme [42] and by expanding the density in atom-centered basis functions, it reaches the remarkable result of being able to make accurate predictions for large molecules, after a training based only on simple compounds (Fig. 1).

Report on milestones

All the milestones for year 5 are progressing on schedule, and for the moment we do not see the need to revise later milestones.

D&D2 — From atoms to additive manufacturing: computational design of complex metal alloys

Project leader: William A. Curtin (EPFL, 2MC)
Computational partners: Michele Ceriotti (EPFL, 1MC), Anatole von Lilienfeld (UniBas)
Experimental partners: Helena Van Swygenhoven (PSI), Christian Leinenbach (Empa)

Status of the project

D&D2 has three major thrusts: the development of first-principles-based machine learning potentials, the application of those potentials to model precipitate evolution in complex alloys, and the prediction of mechanical properties as a function of microstructure evolution.

Considerable progress on machine learning (ML) geared towards complex metallic alloys has been made on three fronts: (1) the application of existing ML frameworks (Behler-Parrinello neural networks (NN) [43]) to a prototypical Al-based alloy [44, 45], (2) the development of machine-learning methods specifically geared towards multi-component systems, e.g. by automatically selecting the most relevant features [46] or by obtaining a low-dimensional representation of the periodic table, to exploit correlations between the behavior of different elements [9]; (3) the development of an efficient and general library to compute representations of atomic environments, and use them to build interatomic potentials.

We have also invested considerable effort in the development of a new fully-consistent DFT database for Al-Mg-Si that is being used to build a new Behler-Parinello-type NN potential. The database is further being extended to include Cu and Zn, with considerable effort devoted so far to obtaining well-converged Cu-Cu interactions in Al. These latter results are relevant for the planned study of Al-Mg-Cu-Zn 7xxx alloys.

Excellent initial progress has also been made on the implementation of a quasi-on-lattice kinetic Monte Carlo (kMC) for precipitate evolution in Al-Mg-Si, using an i-PI code (Fig. 2) [4]. Of particular note is the execution of refined machine learning potentials based on the addition of new structures into the training set as predicted by the kMC model. This was originally envisioned as a key piece of the program, and so this first demonstration is an important

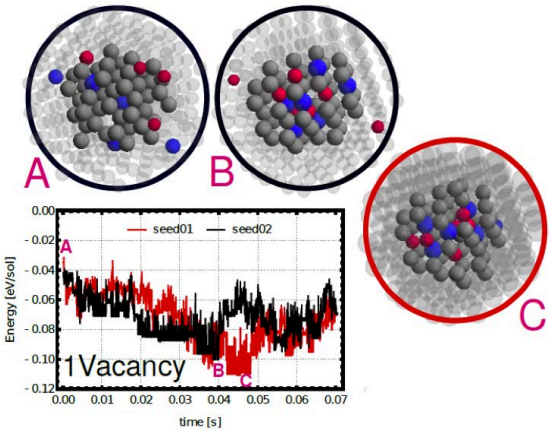

Figure 2: *Early-stage evolution of Al-Mg-Si clusters and total energy during room-temperature natural aging, as computed using kinetic Monte Carlo with our Al-Mg-Si neural network interatomic potential. Blue: Mg atoms; red: Si atoms; dark gray: Al atom neighbors of Mg and Si; light gray: other Al atoms.*

step.

The prediction of mechanical properties has started. We have developed the capability for simulating the misfit-induced stresses caused by cuboidal precipitates of arbitrary dimensions and arbitrary volume fraction. Fundamental atomistic modeling of dislocation core energies and related line tensions is nearly finished. Together, these will provide the first basis for discrete-dislocation-based modeling of the strengthening due to the misfit fields of precipitates.

With the substantial challenge of machine learning potentials for complex alloys, we have also pursued initial application of machine learning potentials to two important elemental metals, Fe and Mg. In collaboration with Csanyi and Marzari, we have completed an evaluation of the double-kink nucleation process for screw dislocations in Fe using the Fe Gaussian Approximation Potential (GAP) [10]. Results show that this potential reproduces all of the physically expected processes that control plasticity in Fe, showing significant improvement over all previous empirical potentials. We have also developed a first Behler-Parinello neural network potential for hcp Mg, a major challenge because of the complexities of dislocation structures in hcp metals. Current results are nearly comparable to the best MEAM-type potential in the literature for Mg, and far better than all existing EAM-type Mg potentials. A second-generation Mg NN potential is being completed now.
We have continued work started under 2017-2018 Agility Plus funding on the DFT-based prediction of strength in high entropy alloys (HEA). Of most importance is a methodology for computing individual atomic misfit volumes in any random HEA. Demonstration of the full computational path in the 6-component fcc RhIrPtPdNiCu alloy shows good contact with the measured yield strength [11]. This predictive capability is being applied to Au-based alloys and to the medium-entropy Ni-Co-Cr alloys that show high strength and extremely high fracture toughness, with preliminary results in good agreement with new experiments.

Report on milestones

The project is on-track for accomplishing the milestones stated in the proposal for year 5, including advanced machine learning of potentials, an operative kMC code, and some initial workflows for metallurgical properties. Work toward some year 6 milestones is well underway.

D&D3 — MARLON: MARVEL Design, Discovery and Engineering of Low-Dimensional Materials and Nanostructures

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

Status of the project

D&D3 is dedicated to the design or discovery of novel low-dimensional materials and nanostructures, and in the engineering and integration of these into novel architectures, devices, and processes. Phase II has seen the inclusion of a new junior PI (Mathieu Luisier, at ETHZ), expert in the computational modeling of complex nanoelectronic devices, of a new female PhD student (Norma Rivano, at EPFL), and the blossoming of experimental collaborations.

The $\sim$ 1800 materials of our *Nature Nanotechnology* paper [12] are being actively screened for properties and performance. For photocatalytic water splitting we identified a promising group of 60 candidates, of which 17 were already known and 47 are novel, and are now being discussed with experimental colleagues (Xile Hu, at EPFL). We have concluded the screening for quantum spin Hall insulators, computing with many-body perturbation theory the inversion strengths of the most promising candidates, thus adding to Jacutingaite [13] a second Kane-Mele candidate and a number of novel QSHIs, including a FET-switchable one. In collaboration with the groups of Alberto Morpurgo and Felix Baumberger at UniGE we have ongoing efforts on the growth and ARPES characterization of 3D samples of Jacutingaite, and with the group of Francesco Stellacci and Harald Brune at EPFL the exfoliation and STM study of the monolayer. We have completed the AiiDA workflows for high-throughput mobilities [14], identified the most promising factors to engineer high-mobility in 2D, and initiated a full screening of the portfolio, while also having completed in collab-

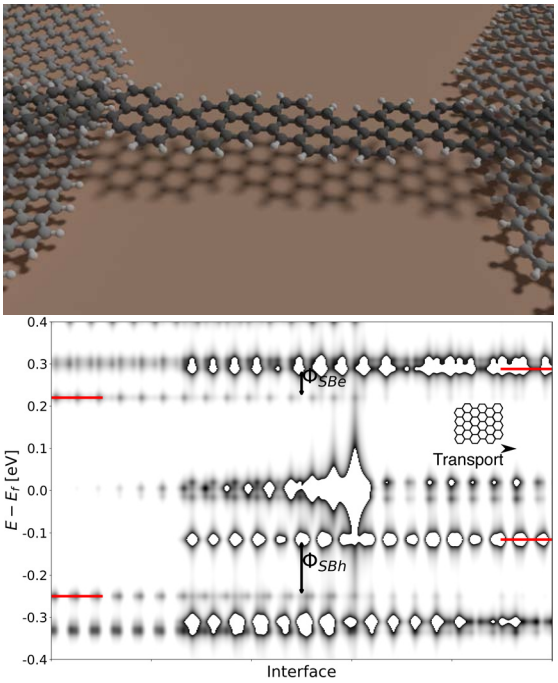

Figure 3: *The figure illustrates the interfacial electronic states of the FET (top panel, currently being built at Empa) for the orientation reported in the inset. The red lines mark the conduction and valence band edges of the lead (left) and the GNR (right). The double ended arrows depicts the Schottky barriers for electrons, Φ_{SBe}, and holes, Φ_{SBh}.*

oration with Andrea Ferrari at the University of Cambridge a paper on the spectroscopic fingerprints of all layered materials, and started developing a *Work* tool for this in the Materials Cloud. We have started, in collaboration with Kumar Agrawal (EPFL), and with a PhD student funded by his chair, a project on gas separation by 2D membranes, focusing first on O_2/N_2 separation in PTI, and in collaboration with Prof. Jonathan Coleman (Trinity College Dublin) a joint experimental-computational effort on describing the size-thickness relationship in liquid-exfoliated nanosheets using non-equilibrium thermodynamics. At the same time we continue the collaboration with Clémence Corminboeuf (EPFL) on the hydrogen evolution reaction, extending it from monolayers to multilayers, and initiated the screening of the portfolio for promising superconductors. Last, we ingested the entire Pauling file, and are working on the overall expansion of the 2D database.

ETH Zurich, in collaboration with EPFL, has focused on the theoretical investigation of logic devices with a single-layer 2D crystal as channel material. The full portfolio has been used as starting point, and the self-consistent calculations have been combined with transformations into maximally localized Wannier functions and fully integrated into ETHZ OMEN quantum transport solver to extract the "current vs voltage" characteristics of various transistor types, materials, and geometries. We started first with band-to-band tunneling transistors (TFETs), identifying several materials that exhibit better performance than transition-metal dichalcogenides (TMDs) due to lower effective masses and band gaps [15, 16]. As next step, the $I-V$ characteristics, injection velocity, and scalability of conventional n- and p-type MOS transistors have been simulated using $\sim$ 100 different 2D monolayers as possible channel materials. The goal of this ongoing activity is to pinpoint compounds with ON-currents that outperform those of Si FinFETs, even down to 5 nm gate lengths. Five to ten such materials have been so far discovered.

Empa is working on a new demonstrator for a "full carbon" FET based on graphene nanoribbons (Fig. 3). After the successful demonstration of synthesis and characterization of GNRs with topologically protected states [17], a low bandgap ribbon has been fabricated and contacted with graphene leads (experiments conducted in collaboration with the group of Prof. Calame at Empa). Characterization of the electronic properties of the leads/ribbon interface is in progress taking into account possible defects on the ribbon and on the leads and the effect of different possible matching geometries between ribbon and contacts. As an example, Fig. 3 shows the interfacial electronic states, band edges, and Schottky barriers for electrons and holes. In collaboration with ETHZ, the transport properties of the device have been computed, and the inclusion of electron-phonon scattering as well as self-consistent calculation of $I-V$ curves at different gate voltages is in progress to support the ongoing experiments on the demonstrator device.

Report on milestones

All of the milestones of the full proposal have been achieved (for the first year), are in progress (for the second year) and broadly speaking have been exceeded.

D&D4 — Nanoporous materials genome: optical, catalytic and electronic properties

Project leader: Berend Smit (EPFL, 2MC)
Computational partners: Jürg Hutter (UZH, 1.5MC), **Alfredo Pasquarello** (EPFL, 1.5MC), **Ivano Tavernelli** (IBM, 1MC)
Experimental partners: Marco Ranocchiari (PSI, 0.33MC + 0.33MC from PSI), **Piero Macchi** (UniBE, 0.33MC), **Kyriakos Stylianou** (EPFL, 0.33MC)

Status of the project

As D&D4 is a novel theme in MARVEL, most groups have started their activities in the beginning of phase II. Several groups have recruited new junior researchers and we are happy to report that by the end of 2018 all groups have their MARVEL team in place.

Synergistic activities

One of the key activities in D&D4 is to develop a set of reference metal-organic frameworks (MOFs) that we use to demonstrate the state-of-the-art in predicting the properties of MOFs. We have carried out the first step in identifying a set of MOFs for each of the domains of interest (gas storage/separations, (photo)catalysis, sensing, etc.) that can serve as a reference. The aim is that by the end of next year we have for each of these materials a full Materials Cloud/AiiDA set of calculations that showcase the current state-of-the-art.
The first step towards this aim is the development of AiiDA workflows which optimize the crystal structure of hypothetical and experimental MOF, and COF (covalent organic framework) structures and assign partial charges to the atoms of a MOF crystal structure. Next, these workflows will be extended to allow for the prediction of adsorption behavior of a large number of gasses.

Current projects

A key component of the activities in D&D4 is the development of efficient methods to compute optical and related properties of MOFs. These activities include:

- Development of fast TDDFT module in CP2K for excited states in MOFs.
- Development of TDDFT based X-ray absorption module in CP2K. Application to the calculation of NEXAFS for MOFs.
- Use of double-hybrid DFT functionals for the accurate calculation of interaction energies of small molecules with MOFs.
- Simulation protocols for the calculation of MOF surface dynamics using force fields and fast quantum chemistry methods.

For screening studies, we are working on more efficient methods to compute optical spectra for large structures like MOFs. The standard approach is GW + Bethe-Salpeter Equation (BSE). We expect that efficiency gains can be made by replacing GW with a hybrid functional calculation. The next step will be to circumvent BSE by using time-dependent DFT on top of hybrid.
Some of the interesting D&D4 results include a methodology to identify zeolite structures from which one can obtain 2-dimensional materials (Fig. 4) and the development of a computational approach to determine whether the addition of functional groups in a MOF can improve the mechanical stability.

Report on milestones

The year 5 milestone was "Make all nanoporous materials available on Materials Cloud." We have uploaded a set of

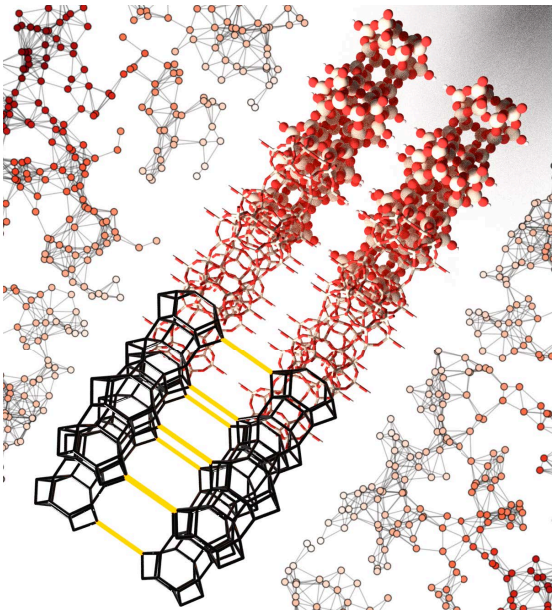

Figure 4: *Examples of 2D zeolite structures.*

ca. 325'000 hypothetical MOF structures and 70'000 hypothetical COF structures on Materials Cloud, which is a fraction of the total number of materials we plan to include. The main reason that we only partially achieved this milestone is that Materials Cloud was originally not designed to handle such large number of materials. These issues have been resolved and in year 6 we expect to have all materials uploaded.

D&D5 — Correlated transition metal oxides and heterostructures

Project leader: Nicola Spaldin (ETHZ, 1MC)
Computational partners: Ulrich Aschauer (UniBE, 1MC), **Claude Ederer** (ETHZ, 1MC), **Philipp Werner** (UniFR, 1MC)
Experimental partners: Marisa Medarde (PSI, 0.5MC + 0.5MC from PSI), Urs Staub (PSI)

Status of the project

We have finalized our implementation of the self-consistent site-dependent DFT+U, charged defect, strain and polarity AiiDA workflows and applied them to $SrMnO_{3-\delta}$ as a test case. We found that self-consistent U parameters lead to an improved description of the bulk structure, while the site dependence leads to significant changes in formation energies [18]. Following this successful test, we started applying the methodology to dopant-vacancy pairs in $SrMnO_3$ to see if this kind of defect cluster can induce polarity, as well as to $LaTiO_3$, to corroborate the DFT+DMFT results obtained at ETH. We further work on an extension of the self-consistent site-dependent approach to DFT+U+V, for the case of strongly covalent materials.

We continued the work on rare earth nickelates, which we started during phase I of MARVEL. We submitted two papers [19, 20], where we demonstrate how the metal-insulator transition (MIT) stabilizes a finite structural distortion in excellent agreement with the experimental data and how this interplay gives rise to a coupled first order electronic-structural transition. We are now performing DFT+DMFT calculations, which also incorporate magnetic order, with the goal of obtaining a complete picture of the nickelates that includes all relevant order parameters.

We have extended our DFT+DMFT studies of oxide heterostructures, publishing a paper describing our earlier results on the effects of strain and finite film thickness on the electronic properties of $CaVO_3$ [21], and preparing one on interfacial effects. Furthermore, we have performed DFT+DMFT calculations for $LaTiO_3/LaVO_3$ multilayers, demonstrating the existence of a metallic interface between these two Mott insulators and showing that its origin suggests the possible design of a Mott transistor.

Motivated by this discovery, we constructed a real-space DMFT model for a slab of $LaVO_3$ sandwiched between $SrTiO_3$ electrodes, and used non-equilibrium DMFT to assess its potential in solar cell applications. We simulated the creation of charge carriers by various photon energies and the transport of these charge carriers to the leads, both in the unbiased polar heterostructure and with an external voltage. We discovered a crucial role of Hund excitations in the harvesting of high-energy photons: in the Mott insulating multi-orbital system, photon energies of the order of 3 eV can excite low-spin configurations, which decay into high-spin configurations and excite additional charge carriers. As a result the optimal gap size of Mott solar cells is smaller ($\sim$ 0.7 eV) than that of semiconductor solar cells ($\sim$ 1.1 eV).

Finally, we explored the effect of correlations on oxygen vacancies in the Mott insulator $LaTiO_3$ and the band insulator $SrTiO_3$ using maximally localized Wannier functions (MLWFs) to construct an effective impurity problem for electrons on the vacancy site, coupled to the usual effective impurity problems on the transition metal sites. Our DFT+DMFT calculations indicate that in $LaTiO_3$ the electrons from the missing oxygen remain bound to the vacancy site (Fig. 5), preserving the Mott insulator, while in $SrTiO_3$ they cause metallic conductivity. In collaboration with the Franchini

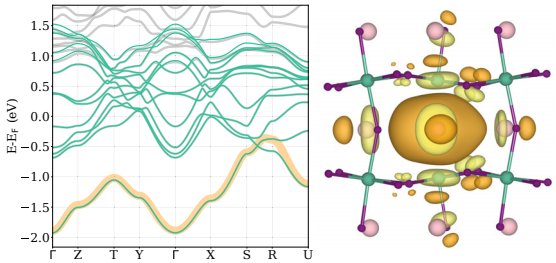

Figure 5: *DFT band structure of $LaTiO_{3-\delta}$ (grey) with MLWF bands superimposed in green. The vacancy band, lying $\sim$ 1.5 eV below E_F, is highlighted and its MLWF shown to the right.*

group at the University of Vienna, we calculated the strength of the screened Coulomb interaction (using the constrained random phase approximation) to estimate the value of U for the vacancy site.

Report on milestones

- *ongoing.* "Identification of the most reliable DFT(+U) or DMFT based approaches to describe point defect-induced properties in transition metal oxides of diverse chemistries".
- *ongoing.* "Perform DFT+DMFT calculations for supercells including point defects material systems close to a Mott MIT in both insulating and metallic regimes. Investigate importance of polaronic relaxations and defect localization".
- *ongoing.* "Identify defects which modify ferroic or electronic properties and incorporate in designer heterostructures".
- *ongoing.* "Identify interface effects between two complex oxides, with one or both components close to a Mott MIT".
- *not yet started.* "Formulate guidelines for the design of specific heterostructures with switchable MITs, suggest candidate materials systems and initiate experimental verification".
- *ongoing.* "Test *ab initio* GW+DMFT scheme on a range of transition metal compounds".
- *updated.* "Test spin-freezing theory of unconventional superconductivity in Sr_2RuO_4 and related compounds. Further develop the ferroelectric quantum critical point mechanism for superconductivity. Identify new materials that optimize either behavior". *Ferroelectric quantum criticality and superconductivity will not be pursued within the MARVEL framework.*
- *ongoing.* "Explore non-equilibrium effects in correlated solids and heterostructures, including Mott solar cells. Test and reveal new strategies for the non-equilibrium design of material properties".

D&D6 — Search for novel topological materials

Project leader: Oleg Yazyev (EPFL, 2MC)
Computational partner: Alexey Soluyanov (UZH, 1MC),
Experimental partner: Ming Shi (PSI, 0.5MC + 0.5MC from PSI), Hugo Dil (EPFL), Christian Rüegg (PSI and UniGE), Arnaud Magrez (EPFL)

Status of the project

Project D&D6 extends the scope of research on topological materials performed during phase I. The results of high-throughput search performed during the first 4 years of MARVEL have now been made publicly available on Materials Cloud as a database with versatile search capabilities. While this TopoMat database is expected to undergo further extension following the progress of D&D6 in phase II, meanwhile we performed detailed investigation of several interesting candidate materials, e.g. the Dirac semimetal $MgTa_2N_3$ with simple band structure [22], and contrarily, a complex gapless topological phase in the nonsymmorphic molecular crystal $OsOF_5$ [23].

Further search and classification of novel topological phases resulted in the discovery of triple-point degeneracies in phonon spectra, that is the realization of bosonic topological phases [24]. Coexistence of these bosonic degeneracies with triple-point electronic counterparts leads to strong thermoelectric response in several materials HfTe, TaSb, TaBi. A homotopy-based theory that extends the tenfold classification of topological materials to include materials that host topological charges forming a non-Abelian group has been developed [25]. We also achieved good progress in classifying composite Weyl nodes (Fig. 6).

Several methodological developments have been carried out during year 5. In particular, the Boltzmann transport approach implemented in the WannierTools code allows to address the physical mechanisms responsible for the extremely large non-saturating magnetoresistances observed in many topological materials [26]. Another development concerns the identification of Fermi-arc surface resonances in topological metals [27]. We have also developed a machine-learning technique for solving the analytics continuation problem that is of direct relevance to correlated materials [28]

As far as experimental activities are concerned, we would like to highlight joint efforts in addressing Coulomb interaction effects in the $MoTe_2$ Weyl semimetal [29, 30], topo-

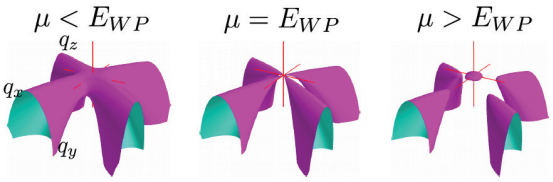

Figure 6: *Evolution of the Fermi surface morphology upon changing chemical potential μ for one of the considered composite Weyl nodes.*

logical interface states in monolayer 1T′-WSe that realizes a quantum spin Hall phase [31], studies of a candidate nodal-line semimetal CaAgP [32] and ferromagnetic Kagome-lattice material Fe_3Sn_2 that hosts topological degeneracies [47].

Good progress in adopting the methodologies suitable to treating correlated topological materials has been achieved. In collaboration with the group of Xi Dai, we started a project on addressing the origin of quantum oscillations in SmB_6 and YbB_{12} using DMFT, while Gutzwiller approximation was used to study excitonic magnetism in topological iridate $Ba_3CaIr_2O_9$. We have also initiated a work on the design of interacting topological phases in twisted bilayer 2D materials. Finally, significant progress have been achieved in identifying new Co-based ($3d^7$) candidate materials for realizing the Kitaev model.

Report on milestones

During year 5 significant progress has been achieved with regard to two milestones. DMFT and Gutzwiller methodologies have been adopted to study selected topological materials ($Ba_3CaIr_2O_9$, SmB_6), and further extension of this research line is expected. The milestone foreseen for year 5 is largely achieved. In addition, two Co-based Kitaev model materials have been identified, thus implying a significant progress towards a milestone originally planned for year 7.

Inc1 — Design and discovery of novel solid-state ionic conductors

Project leader: Teodoro Laino (IBM, 1MC)
Computational partner: Nicola Marzari (EPFL, 1MC)
Experimental partners: Daniele Pergolesi (PSI, 0.5MC + 0.5MC from PSI), **Claire Villevieille** (PSI, 0.5MC + 0.5MC from PSI)

The primary goal of this MARVEL incubator is the discovery of novel solid-state electrolytes (SSE) for next-generation batteries technology achieving higher energy density, power density and safety compared to commercial counterparts. It builds upon phase I computational results (**EPFL** and **IBM**), and aims in phase II at device level prototyping thanks to the synergy with experimental groups at **PSI**.

Status of the project

The screening of all Li-containing compounds without partial occupations in the ICSD [48] and COD [49] via the AiiDA platform was concluded during Q2 2018. The pinball model [33], direct output of phase I (**EPFL**), was used as a first screening step to find ion-conducting structures among 1'300 candidates. First-principles molecular dynamics (FPMD) simulations were performed for the best 130 candidates. Two of them (Li_7TaO_6 (LTO) and $Li_{10}GeP_2O_{12}$ (LGPO)) were chosen as first promising candidates for experimental synthesis and characterization (**PSI**).

Both LTO and LGPO showed relevant Li-ion conductivity, measured by impedance spectroscopy (see, e.g., inset bottom left in Fig. 7); the crystal structure and absence of secondary phases was determined by X-ray diffractometry.

The first experimental characterization (**PSI**) of LTO and aliovalent substitutions with Zr^{4+} and

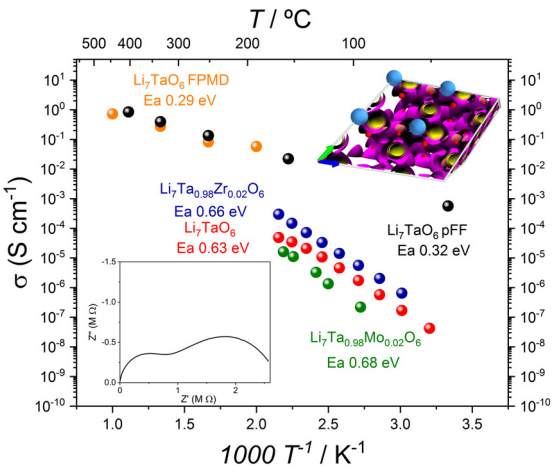

Figure 7: *Conductivity of LTO from experiments (with aliovalent substitutions) and simulations (FPMD and pFF). Top right: Lithium probability density distribution from simulations. Bottom left: Nyquist diagram from impedance spectroscopy.*

Mo^{6+} produced a lower conductivity than inferred from FPMD (**EPFL**), motivating the application of polarizable force-field (pFF) simulations (**IBM**), to test the material behavior at greater time and length scales. Results from different simulations and experiments are compared in Fig. 7. The agreement between pFF and FPMD clearly suggests that LTO samples can be further optimized, and different synthesis and sintering procedures are currently under investigation.

LGPO was synthesized (**PSI**) in its orthorhombic phase, the measured conductivity agreeing with the values computed from FPMD (**EPFL**). Similar to $Li_7LaZr_2O_{12}$, LGPO is predicted to have a highly conductive phase (tetragonal), which happens to be less stable and whose stabilizing conditions are still to be identified.

Beyond the synergies between experiments and simulations, several novel computational tools are under development: a method for automatically detecting low-energy sites from molecular dynamics simulations (**EPFL**); an AiiDA workflow to compute the electrochemical stability window of a SSE, complementary to the grand-potential phase diagram method (**IBM**) [50]; an AiiDA-based infrastructure for fitting pFFs (**IBM**) [34]. In addition, the team is exploring applications of neural network architectures to the simulation of SSE (**IBM**).

Report on milestones

M1: Milestone achieved. Screened all Li-containing compounds in the ICSD and COD via DFT band-gaps and an estimate of the lithium-ion diffusion in the pinball model.

M7: Milestone achieved. Completed FPMD simulations and calculated diffusion coefficients for 130 materials at high temperature.

Inc2 — Active machine learning for computational materials design

Project leader: Anatole von Lilienfeld (UniBas, 1.5MC)
Computational partners: Volker Roth (EPFL, 1MC), Michele Ceriotti (EPFL), Martin Jaggi (EPFL)

Status of the project

Latent representations of molecules.

The *inverse problem* of materials design, i.e. predicting compounds is a well-known and hard problem since it reverses the causal direction of quantum mechanical calculations. One of the key aspects for solving the inverse problem is the search for "simple" molecule representations that capture all relevant compositional and configurational variables defining the molecule as well as all structural design constraints for generating new valid molecules. Therefore, we are focusing on the development of machine learning models that automatically learn such latent molecule representations from data.

We have started with deep neural network architectures of *information bottleneck* type which aim at finding a low-dimensional and structured representation of molecules inside a generative probabilistic model from which we can *jointly* sample new molecules and their properties. These models are composed of two submodules: an *encoder* associates each molecule with a coordinate value in a continuous latent space, and a *decoder* maps each such coordinate value to a molecule and a specific combination of molecular properties. An illustration is given in Fig. 8 (left).

Response properties

Further progress has been made in extending and improving the applicability of quantum machine learning (QML) models of quantum properties of materials and molecules [36]. Based on an improved representation of atoms in their environment for use in quantum machine learning (QML) models [36], and used in conjunction with simple kernel ridge regression (KRR) machine learning approach, we have demonstrated unprecedented predictive power for several benchmark dataset [36]. We have then expanded the applicability of this machine learning approach by explicitly including the physically correct property depen-

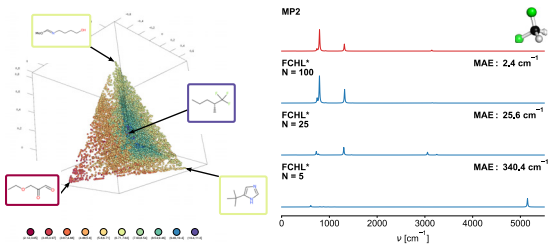

Figure 8: *Left: "deep chemical archetypes" in latent space in terms of HOMO-LUMO gap energy. Right: Machine learning based predictions (blue) and MP2 reference (red) infrared spectrum of dichloromethane for training set sizes ($N = 5, 25, 100$) [35].*

dency in the representation. More specifically, we have developed a new machine learning formalism that builds on the concept of response operators [35]. The response operator formalism is up to $10-100\times$ faster than conventional Gaussian Process Regression of response properties, and it reduces memory requirements ten-fold. We have numerically demonstrated that the formalism reproduces atomic forces and harmonic frequency with state-of-the-art accuracy, as well as electric-field dependent properties such as dipole moments for which the method reduces the amount of required training data by up to 20 times when compared to previously established methods. Fig. 8 illustrates the applicability of the method to the prediction of infrared spectra.

Report on milestones

Work on milestone 1 "ML models for selecting typical compounds and for learning representations through latent variable models" and milestone 2 "Improved learning curves" has started (see also [35]). Some developments have already been made available through open source software QMLcode-package maintained at GitHub. We anticipate that these implementations will be useful for any MARVEL projects that can profit from machine learning techniques. Work on milestones 3 "Active learning" and 4 "Inclusion of archetypes and learned representations" has not yet begun.

OSP — Open science platform

Project leader: Giovanni Pizzi (EPFL)

Status of the project

AiiDA

AiiDA core Most of the work focused on preparing the next major release (1.0, scheduled in the first half of 2019; 4 alpha versions are already out), with over 1'500 commits on top of v0.12 (stable, maintained with bugfixes and backports, and used in production). Work performed in year 5 (already included into the 1.0 alpha releases) includes a new event-based daemon and workflow engine based on Circus and RabbitMQ; additional features to the workflow engine to facilitate reuse of common code; a complete rewrite of the command-line interface, facilitating automated testing; full Python 2/3 support; speed optimizations for the JSONB database backend; a major reorganization of the node hierarchy and the provenance model that simplified and defined formally AiiDA's provenance ontology; code reorganization to stabilize the Python API. These changes came with sophisticated automated migrations to support users in the few cases when back-compatibility was impossible.

AiiDA plugins Since the deployment of the AiiDA plugin registry, there are now 27 plugin entries supporting 59 codes and 51 workflows. Plugins are now being contributed also by non-MARVEL researchers, but many plugins (e.g. for the codes qeq, ddec, raspa, gudhi) have been implemented specifically for the needs of MARVEL groups. Moreover, significant improvements have been done to existing plugins (e.g. Quantum ESPRESSO, CP2K) to develop robust workflows (cell/geometry optimization, molecular dynamics) and to support specific workflow needs in MARVEL groups.
Plugin development has been simplified by a scaffolding "cookiecutter" recipe (working both with Python 2/3 and AiiDA 0.12 and 1.0) to kickstart a new plugin, while a workshop (scheduled in Mar 2019) will support existing plugin developers in migrating to AiiDA 1.0 and Python 3. Finally, the AiiDA calculation examples for Quantum ESPRESSO and CP2K have been converted into web demos requiring no installation, using Binder [51].

Materials Cloud

Materials Cloud acts as the web platform of the MARVEL OSP [37, 38]. Materials Cloud *Learn* continues to grow with all MARVEL distinguished lectures. Web tools in the *Work* section increased from 1 to 4, including fast and reliable machine-learned models predicting advanced materials properties. The Jupyter section is now called AiiDA Lab and developing new apps is now facilitated by our library of common widgets to support common AiiDA functionality, and new widgets to support periodic tables and directed graphs. Furthermore, we have started the integration with the EUDAT B2ACCESS service, paving the way to the integration of AiiDA Lab in, e.g., the European Open Science Cloud. The Quantum Mobile virtual machine has been modularized for easier maintainability and reuse, and various

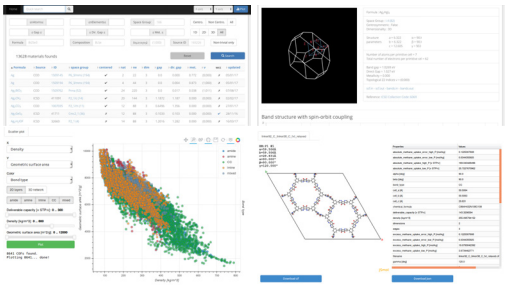

Figure 9: *Screenshots of some of the new* Discover *sections of Materials Cloud: the topological materials screening (top, ∼ 14′000 materials) and the covalent organic frameworks (COFs) optimized for methane storage applications (bottom, ∼ 70′000 materials).*

different versions can now be created seamlessly. Quantum Mobile has been used for over five courses and tutorials and successfully deployed on VirtualBox, AWS and OpenStack. New versions are being released regularly, the most recent with updated OS (Ubuntu 18.04) and codes. Two new curated datasets, contributed by two different groups (Smit and Yazyev), enrich the *Discover* section (Fig. 9) with thousands of new systems (topological materials and covalent organic frameworks). The *Archive* section, now registered on FAIRsharing and a recommended data repository by the *Nature*'s journal *Scientific Data*, continues to attract new data entries. New contributions have been streamlined thanks to an upload form and clear moderation policies. Moreover, metadata is now published using standard formats (Dublin Core, schema.org). Finally, on the technical side, the deployment of the platform has been simplified via improved ansible scripts and an external server now provides continuous monitoring of the status of the whole infrastructure.

Report on milestones

"Stabilisation of AiiDA, code optimisation": on track (new fast event-based daemon implemented, AiiDA v1.0 release expected in first half of 2019). "Support in AiiDA for codes used in MARVEL": achieved (6 new codes: ddec, gudhi, phtools, qeq, raspa, zeopp; and continuous improvement of existing plugins: Quantum ESPRESSO, CP2K, etc.). "Development of turn-key solutions": on track (linear response phonon workflows for Quantum ESPRESSO available). "Data management plan templates for SNSF": achieved (available on Materials Cloud). "Release of an embedding protocol based on Docker containers for Materials Cloud tools": on track (tools-barebone implemented, current tools being migrated to it). "Creation of an AiiDA Lab App Store": on track (app registry implemented, with 14 apps already registered). "Keep increasing the number of curated datasets and computed properties": on track (two new *Discover* sections; Pauling File contract signed, ∼ 100′000 SCF calculations using SIRIUS already performed).

HPC — HPC and future architectures

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

Status of the project

The project HPC and Future Architectures supports the deployment of the next hardware resource for MARVEL, located at CSCS, and hence it is mostly an equipment effort, with a significant element of software co-design, to ensure that there is convergence on an optimal hardware and software roadmap. This project ensure the availability of a GPU enabled PW library (SIRIUS) for the MARVEL community. For the first year of the second phase the following tasks were set: working, validated and tested implementation of SIRIUS working with Quantum ESPRESSO (pseudopotentials) and Exciting (all-electron full potential), for the calculation of total energies, forces, and stresses in non-magnetic systems. The tasks have made good progress to the extent that the software is available to users on the system in a beta state, and delivers an over two-fold speedup for systems on medium size. A paper is in preparation.

Report on milestones

Fortran API of the SIRIUS domain-specific library has been stabilized and the integration of the SIRIUS library in Quantum ESPRESSO and Exciting codes was finished.
For the Quantum ESPRESSO (QE) code, an additional Fortran module file was added to handle exchange of parameters and data between the two codes. This approach minimizes the amount of modification in the QE baseline code, facilitates maintenance, and allows easy integration of current or future features supported by SIRIUS. An EasyBuild recipe for the QE+SIRIUS code was added to the list

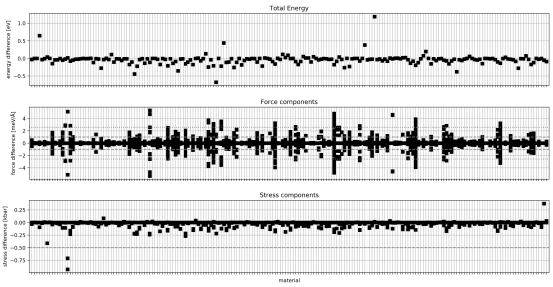

Figure 10: *Comparison of the total energies, forces and stress tensor components performed on 524 non-magnetic structures using the conventional and SIRIUS-enabled* Quantum ESPRESSO *codes.*

of production applications at CSCS. The users of Piz Daint are now provided with a GPU-accelerated QE code.

The Exciting code was adjusted to use the new Fortran API of SIRIUS and the performance of the Exciting+SIRIUS code was verified. Work is in progress to include the Exciting code modifications in the official version.

For the plane wave pseudopotential codes, SIRIUS library provides the functionality to compute ground state, atomic forces and stress tensor for the non-magnetic materials. The library also includes prototyping code for collinear and non-collinear magnetic systems, spin-orbit and Hubbard interactions, as well as force and stress corrections associated to these interactions. The prototype code is already functional but further testing and improvements are needed before the official release.

In collaboration with the group of Nicola Marzari at EPFL we tested integration of the SIRIUS library in QE and interaction with the AiiDA framework on a set of $\sim$ 500 non-magnetic crystal structures for which the total energy, forces and stresses were computed. The results (Fig. 10) show a good agreement between the two codes. The small difference in results was tracked down to different radial integration schemes implemented in SIRIUS (cubic splines) and in QE (Simpson's integration). This difference is small and does not affect the validity of results.

The SIRIUS library can also be used to compute the DFT properties of magnetic systems, but calculating the DFT ground state can be very challenging with conventional iterative solver methods. To address this problem, we started to implement more robust methods for insulators and metals using the Python API included in the library. Development is progressing rapidly and eventually all this work will be integrated in the C++ code base of the library.

MARVEL publications

[1] A. Fabrizio, B. Meyer, C. Jeanguenat, and C. Corminboeuf, the title for now is *OASIS-16: a benchmark set of organic molecular crystal semiconductors, in preparation* (2019).

[2] P. M. Piaggi, O. Valsson, and M. Parrinello, *Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations*, Physical Review Letters **119**, 015701 (2017).

[3] P. M. Piaggi and M. Parrinello, *Predicting polymorphism in molecular crystals using orientational entropy*, Proceedings of the National Academy of Science of the USA **115**, 10251 (2018).

[4] V. Kapil, M. Rossi, O. Marsalek, R. Petraglia, Y. Litman, T. Spura, B. Cheng, A. Cuzzocrea, R. H. Meißner, D. M. Wilkins, B. A. Helfrecht, P. Juda, S. P. Bienvenue, W. Fang, J. Kessler, I. Poltavsky, S. Vandenbrande, J. Wieme, C. Corminboeuf, T. D. Kühne, D. E. Manolopoulos, T. E. Markland, J. O. Richardson, A. Tkatchenko, G. A. Tribello, V. V. Speybroeck, and M. Ceriotti, *i-PI 2.0: A universal force engine for advanced molecular simulations*, Computer Physics Communications (2018), doi:10.1016/j.cpc.2018.09.020.

[5] 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).

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

[7] A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti, *Transferable Machine-Learning Model of the Electron Density*, ACS Central Science **5**, 57 (2019).

[8] L. Vannay, B. Meyer, R. Petraglia, G. Sforazzini, M. Ceriotti, and C. Corminboeuf, *Analyzing Fluxional Molecules Using DORI*, Journal of Chemical Theory and Computation **14**, 2370 (2018).

[9] M. J. Willatt, F. Musil, and M. Ceriotti, *Feature Optimization for Atomistic Machine Learning Yields a Data-Driven Construction of the Periodic Table of the Elements*, Physical Chemistry Chemical Physics **20**, 29661 (2018).

[10] F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin, *Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential*, npj Computational Materials **4**, 69 (2018).

[11] B. Yin and W. A. Curtin, *First-principles-based prediction of yield strength in the RhIrPdPtNiCu high entropy alloy*, npj Computational Materials **5**, 14 (2019).

[12] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Nature Nanotechnology **13**, 246 (2018).

[13] A. Marrazzo, M. Gibertini, D. Campi, N. Mounet, and N. Marzari, *Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator*, Physical Review Letters **120**, 117701 (2018).

[14] T. Sohier, D. Campi, N. Marzari, and M. Gibertini, *Mobility of two-dimensional materials from first principles in an accurate and automated framework*, Physical Review Materials **2**, 114010 (2018).

[15] Á. Szabó, C. Klinkert, D. Campi, C. Stieger, N. Marzari, and M. Luisier, *Ab Initio Simulation of Band-to-Band Tunneling FETs With Single- and Few-Layer 2-D Materials as Channels*, IEEE Transactions on Electron Devices **65**, 4180 (2018).

[16] C. Klinkert, A. Szabo, D. Campi, C. Stieger, N. Marzari, and M. Luisier, *Novel 2-D Materials for Tunneling FETs: an Ab-initio Study*, in *2018 76th Device Research Conference (DRC)* (IEEE, 2018), pp. 1–2.

[17] O. Gröning, S. Wang, X. Yao, C. A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Müllen, P. Ruffieux, and R. Fasel, *Engineering of robust topological quantum phases in graphene nanoribbons*, Nature **560**, 209 (2018).

[18] C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer, *Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$*, arXiv:1811.10858 (2018).

[19] A. Hampel, P. Liu, C. Franchini, and C. Ederer, *Energetics of the coupled electronic-structural transition in the rare-earth nickelates*, arXiv:1807.03524 (2018).

[20] O. E. Peil, A. Hampel, C. Ederer, and A. Georges, *Mechanism and control parameters of the metal-insulator transition in nickelates*, arXiv:1809.03720 (2018).

[21] S. Beck, G. Sclauzero, U. Chopra, and C. Ederer, *Metal-insulator transition in $CaVO_3$ thin films: Interplay between epitaxial strain, dimensional confinement, and surface effects*, Physical Review B **97**, 075107 (2018).

[22] Q. Wu, C. Piveteau, Z. Song, and O. V. Yazyev, *$MgTa_2N_3$: A reference Dirac semimetal*, Physical Review B **98**, 081115(R) (2018).

[23] H. Lee and O. V. Yazyev, *Plethora of Coexisting Topological Band Degeneracies in Nonsymmorphic Molecular Crystal $OsOF_5$*, arXiv:1808.06346 (2018).

[24] S. Singh, Q. Wu, C. Yue, A. H. Romero, and A. A. Soluyanov, *Topological phonons and thermoelectricity in triple-point metals*, Physical Review Materials **2**, 114204 (2018).

[25] Q. Wu, A. A. Soluyanov, and T. Bzdušek, *Beyond the Tenfold Way: Non-Abelian Topology in Noninteracting Metals*, arXiv:1808.07469 (2018).

[26] S. Zhang, Q. Wu, Y. Liu, and O. V. Yazyev, *Magnetoresistance from Fermi Surface Topology*, Physical Review B **99**, 035142 (2019).

[27] D. Gosálbez-Martínez, G. Autès, and O. V. Yazyev, *Topological Fermi-arc surface resonances in bcc iron*, arXiv:1811.08178 (2018).

[28] R. Fournier, L. Wang, O. V. Yazyev, and Q. Wu, *An Artificial Neural Network Approach to the Analytic Continuation Problem*, arXiv:1810.00913 (2018).

[29] N. Xu, Z. W. Wang, A. Magrez, P. Bugnon, H. Berger, C. E. Matt, V. N. Strocov, N. C. Plumb, M. Radovic, E. Pomjakushina, K. Conder, J. H. Dil, J. Mesot, R. Yu, H. Ding, and M. Shi, *Evidence of Coulomb-interaction-induced Lifshitz transition and robust hybrid Weyl semimetal in T_d-$MoTe_2$*, Physical Review Letters **121**, 136401 (2018).

[30] A. P. Weber, P. Rüßmann, N. Xu, S. Muff, M. Fanciulli, A. Magrez, P. Bugnon, H. Berger, N. C. Plumb, M. Shi, S. Blügel, P. Mavropoulos, and J. H. Dil, *Spin-resolved electronic response to the phase transition in $MoTe_2$*, Physical Review Letters **121**, 156401 (2018).

[31] M. M. Ugeda, A. Pulkin, S. Tang, H. Ryu, Q. Wu, Y. Zhang, D. Wong, Z. Pedramrazi, A. Martín-Recio, Y. Chen, F. Wang, Z.-X. Shen, S.-K. Mo, O. V. Yazyev, and M. F. Crommie, *Observation of topologically protected states at crystalline phase boundaries in single-layer WSe_2*, Nature Communications **9**, 3401 (2018).

[32] N. Xu, Y. T. Qian, Q. S. Wu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, V. N. Strocov, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, O. V. Yazyev, T. Qian, H. Ding, J. Mesot, and M. Shi, *Trivial topological phase of CaAgP and the topological nodal-line transition in $CaAg(P_{1-x}As_x)$*, Physical Review B **97**, 161111(R) (2018).

[33] L. Kahle, A. Marcolongo, and N. Marzari, *Modeling lithium-ion solid-state electrolytes with a pinball model*, Physical Review Materials **2**, 065405 (2018).

[34] M. Mottet, T. Binninger, A. Marcolongo, and T. Laino, *zrl-aiida-toolbox* (2018), https://github.com/zrl-aiida-toolbox/zrl-aiida-toolbox.

[35] A. S. Christensen, F. A. Faber, and O. A. von Lilienfeld, *Operators in quantum machine learning: Response properties in chemical space*, The Journal of Chemical Physics **150**, 064105 (2019).

[36] F. A. Faber, A. S. Christensen, B. Huang, and O. A. von Lilienfeld, *Alchemical and structural distribution based representation for universal quantum machine learning*, The Journal of Chemical Physics **148**, 241717 (2018).

[37] G. Pizzi, A. Togo, and B. Kozinsky, *Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath*, MRS Bulletin **43**, 696 (2018).

[38] G. Pizzi, *Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud*, in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. Andreoni and S. Yip, eds. (Springer, Cham, 2018), pp. 1–24.

Other references

[39] B. Cheng and M. Ceriotti, *Computing the absolute Gibbs free energy in atomistic simulations: Applications to defects in solids*, Physical Review B **97**, 054102 (2018).

[40] B. Cheng, A. T. Paxton, and M. Ceriotti, *Hydrogen Diffusion and Trapping in α-Iron: The Role of Quantum and Anharmonic Fluctuations*, Physical Review Letters **120**, 225901 (2018).

[41] M. Ropo, M. Schneider, C. Baldauf, and V. Blum, *First-principles data set of 45,892 isolated and cation-coordinated conformers of 20 proteinogenic amino acids*, Scientific Data **3**, 160009 (2016).

[42] A. Grisafi, D. M. Wilkins, G. Csányi, and M. Ceriotti, *Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems*, Physical Review Letters **120**, 036002 (2018).

[43] J. Behler and M. Parrinello, *Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces*, Physical Review Letters **98**, 146401 (2007).

[44] R. Kobayashi, D. Giofré, T. Junge, M. Ceriotti, and W. A. Curtin, *Neural network potential for Al-Mg-Si alloys*, Physical Review Materials **1**, 053604 (2017).

[45] D. Giofré, T. Junge, W. A. Curtin, and M. Ceriotti, *Ab initio modelling of the early stages of precipitation in Al-6000 alloys*, Acta Materialia **140**, 240 (2017).

[46] G. Imbalzano, A. Anelli, D. Giofré, S. Klees, J. Behler, and M. Ceriotti, *Automatic selection of atomic fingerprints and reference configurations for machine-learning potentials*, The Journal of Chemical Physics **148**, 241730 (2018).

[47] M. Yao, H. Lee, N. Xu, Y. Wang, J. Ma, O. V. Yazyev, Y. Xiong, M. Shi, G. Aeppli, and Y. Soh, *Switchable Weyl nodes in topological Kagome ferromagnet Fe_3Sn_2*, arXiv:1810.01514 (2018).

[48] A. Belsky, M. Hellenbrandt, V. L. Karen, and P. Luksch, *New developments in the Inorganic Crystal Structure Database (ICSD): accessibility in support of materials research and design*, Acta Crystallographica B **58**, 364 (2002).

[49] 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).

[50] M. Nakayama, M. Kotobuki, H. Munakata, M. Nogami, and K. Kanamura, *First-principles density functional calculation of electrochemical stability of fast Li ion conducting garnet-type oxides*, Physical Chemistry Chemical Physics **14**, 10008 (2012).

[51] Project Jupyter, Matthias Bussonnier, Jessica Forde, Jeremy Freeman, Brian Granger, Tim Head, Chris Holdgraf, Kyle Kelley, Gladys Nalvarte, Andrew Osheroff, M. Pacer, Yuvi Panda, Fernando Perez, Benjamin Ragan-Kelley, and Carol Willing, *Binder 2.0 - Reproducible, interactive, sharable environments for science at scale*, in *Proceedings of the 17th Python in Science Conference*, Fatih Akici, David Lippa, Dillon Niederhut, and M. Pacer, eds. (2018), pp. 113 – 120.

1.2 Structure

In phase II, MARVEL is organized around 6 Design & Discovery projects (major collaborative projects covering key topics in energy, ICT, manufacturing, and pharma, and ranging from molecular crystals to complex metal alloys to topological materials), 2 Incubator projects (more focused efforts, dedicated presently to solid-state ionic conductors and machine learning). In addition, 2 core structural efforts are represented by the Open Science platform (which provides open access to simulation services and tools, dissemination and preservation of curated and raw data, and educational material) and the HPC and Future Architectures platform, which supports the deployment of the next hardware resources for MARVEL, and the co-design of software and hardware.
EPFL is the home institution and participating scientists are affiliated with 11 Swiss academic and industrial institutions.
In phase II, along with the director, Nicola Marzari, Berend Smit (EPFL) is deputy director, and Clémence Corminboeuf (EPFL) and William Curtin (EPFL) complete the executive committee in charge of day-to-day activities. Strategic decisions are taken by an enlarged committee counting also Alfredo Pasquarello (EPFL), Thomas Schulthess (CSCS and ETHZ) and Frithjof Nolting (as representative of PSI).
In the management team, Patrick Mayor joined as program manager at 60% from Sep 2018, following Nathalie Jongen's departure; Patrick brings extensive experience as coordinator of the Swiss Nano-Tera.ch program. Carey Sargent increased her work percentage from 20%, dedicated to technology transfer, to 40% from Oct 2018 for the coverage of MARVEL-related news and to reinforce the communication team, complemented by freelance scientific journalist Fiorien Bonthuis. Finally, Cornelia Bujenita is the new administrative assistant from Jan 2019, replacing Sonia Collaud.

1.3 Strategies

Knowledge and technology transfer

Knowledge transfer

Software

The advancements in AiiDA (Fig. 11), Materials Cloud or the Quantum Mobile virtual machine have already been described in the OSP section, p. 12. An interesting educational outcome of these KTT activities can be seen in the Quantum Mobile - this was used in school and classes, going from the online classes of Prof. S. Cottenier compmatphys.epotentia.com to the "MolSim-2019: Understanding Molecular Simulation" school in Amsterdam (Jan 2019, Prof. B. Smit) to the ASESMA-2018 school in Addis Ababa (Oct 2018, Prof. S. Narasimhan). Notably, a 2-year project to support the scalability of Materials Cloud and involving 5 MARVEL PIs was recently funded by swissuniversities P5; this will support 2+ FTEs for the next 2 years to scale the reach of the Materials Cloud to several other communities in physics, chemistry and engineering.

Collaborations and conferences

MARVEL is actively engaged in several H2020 European projects: a core collaboration involving the Materials Cloud will take place through phase 2 (2019-21) of the MaX Centre of Excellence, that is the sole H2020 Centre dedicated to HPC and materials. In addition to the ongoing efforts in the theory, simulation, and data pillars of the Nanoscience Foundries & Fine Analysis (NFFA), and the coordination and support action for the European Materials Modelling Council (EMMC), we highlight the MarketPlace project (2018-22), dedicated to providing a single-stop solution for European industry interested in simulations and data, and the INTERSECT project (2019-21), to interface proprietary device modeling codes with open-source efforts like Quantum ESPRESSO and SIESTA, using AiiDA as the backbone.
MARVEL members organized or co-organized more than 20 conferences, tutorials and workshops. We can mention dedicated sessions at PASC 2018 and at the Annual Meeting of the Swiss Physical Society. All are listed in the NIRA database and on the website.

Technology transfer

This year, we have reinforced the contacts with the industrial community with the setup of an Industrial Advisory Board (IAB) representing the 5 industrial sectors covered by MARVEL research (metals, chemicals, ICT, energy, pharma). This consultative group is chaired by Erich Wimmer, CEO of Materials design. Participants are all C-level or senior people: F. Diologent (Richemont), T. Eckl (Robert Bosch), A. Ryoji (Toyota R&D Central Labs), N. Cudré-Mauroux (Solvay) and A. Grandeury (Novartis). A 1-day meeting has been organized in Sep 2018 during the Review and Retreat, with all the members in attendance. The next step is the organization of Industry Sector Days, as

Figure 11: *From left to right: third AiiDA coding week in the Swiss Alps, Dec 2018. CCMX – MARVEL Materials Science Day, Bern, Oct 2018. MARVEL Junior Retreat, Fieschertal, Jul 2018. International Workshop on Computational Design and Discovery of Novel Materials COMDI 2018, EPFL, Sep 2018.*

planned in our phase II TT strategy. The first one on metals will take place on 15 Feb 2019 with 6 guest industries and 4 PIs. Next ones in chemistry, pharma, new electronics and energy are now being prepared. The IAB is of great help for the choice of the topics and the selection of the industrial participants. The CCMX – MARVEL Materials Science Day took place in Bern on 4 Oct 2018, with around 70 participants, among them 25 industry representatives from Swiss watchmaking, medtech and metallurgy sectors (Fig. 11).
A core achievement for this year has been the signature of a general collaboration protocol and 2 research agreements with a large European company active in materials and chemicals, for a total amount of 1.5 MCHF. In parallel, the watch-making company financing a PhD since 2014 has decided to extend the collaboration by a year, and is exploring further collaborations. Two patents have been filed by MARVEL PIs.
Our industrial community, composed of 56 companies by the end of 2017 has been enlarged with 10 new companies having received general information from the tech transfer officer during meetings. 6 other new companies paid a first visit to one or several MARVEL PIs. With 4 of them, scientific discussions are open for potential collaboration. Subscriptions to the industrial newsletter rose to 153 from 80 since its first introduction in Nov 2017.

Education and training

PhD students and postdoctoral researchers

The 4-day MARVEL Junior Retreat took place on 17 – 20 Jul 2018 in Fieschertal (Fig. 11) and was attended by 33 participants from the MARVEL community (15 postdocs, 13 PhD students and 5 INSPIRE Potentials Master's students). The event, organized by 2 junior researchers, was planned in a workshop style including selected keynote speeches aimed at improving research skills and professional development, and presentations by the participants, carefully chosen to achieve a good balance of research groups, gender, as well as master students, PhDs and postdocs. Other activities were organized in order to foster friendly relations between different groups in the community.
Dr. Gareth Tribello (Queen's Univ. Belfast) gave a workshop "Writing a good paper" to MARVEL PhD students and postdocs on 5 Jul 2018. MARVEL distinguished lectures are filmed and made available on the *Learn* platform of Materials Cloud. MARVEL sponsored the 5^{th} African School on Electronic Structure Methods and Applications ASESMA-2018, Addis Ababa, Ethiopia, 22 Oct – 2 Nov 2018 and sent 3 people as mentors (Fig. 12).

Younger generation

MARVEL, with the support of the EPFL high-performance computing team SCITAS, has organized the first edition of a 2-week summer camp (25 Jun – 6 Jul 2018) for high school students, in which 13 of them could learn the basics of programming to study materials (Fig. 12). During the camp, they were introduced to the fundamentals of programming and key physics principles before tackling their first hands-on exercises related to materials science and realizing a concrete project. The feedback was overwhelmingly positive: despite finding the topics and exercises challenging, the participants enjoyed the opportunity to learn new concepts and to get a first glimpse of the research world through the lab visits and the interactions with PhD students and postdocs. A similar camp is being organized for the summer 2019, over 1 week without the project part.

Equal opportunities

Equal opportunities analysis and plans

We summarize hereafter the activities that have taken place in year 5, but for our full strategy, plans and efforts see *Annex 2 NCCR MARVEL year 5 — Equal opportunities, analysis and plans*, submitted in Jan 2019 to SNSF.

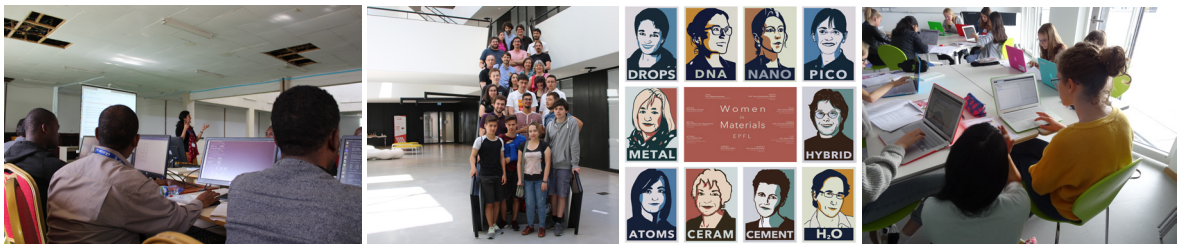

Figure 12: *From left to right: ASESMA-2018, Addis Ababa, Oct-Nov 2018. Summer camp for high school students, EPFL, Jun-Jul 2018. The new installation in the entrance of the Institute of Materials promoting EPFL women professors in materials, unveiled Nov 2018.* Coding club des filles, *EPFL, Oct 2018.*

Gender trainings

MARVEL now offers all its members a 3-hour training focused on gender and ethical/respectful behavior coordinated by Prof. Marianne Schmid Mast, Chair of Organizational Behavior at the Faculty of Business and Economics (HEC) of UniL. Concretely, 2 training sessions on "Overcome implicit bias in recruiting and supervising a diverse workforce" will be organized for MARVEL PIs at EPFL on 14 May and in Zurich on 25 May 2019. An additional series of trainings entitled "Beyond bias: Diversity and team work" will be dedicated to PhD students and postdocs, by groups of $12-15$ people. The first 2 sessions will take place on 3 Jun at EPFL and 4 Jun in Zurich.

INSPIRE Potentials fellowships

With 2 calls in 2018, 7 new students were granted an INSPIRE Potentials — MARVEL Master's fellowship to conduct a 6-month research in a computational lab belonging to MARVEL. From 2019, all the new fellows are offered a mentoring scheme. In total 21 students received a grant for a Master's project in 12 different MARVEL groups in 6 institutions. The full list can be found here.

Events

- MARVEL female researchers were directly informed about a dozen dedicated activities (lunch events, conferences or workshops) organized in 2018 at EPFL or in other participating institutions.
- MARVEL encourages its female PhD students and postdocs to participate in training, mentoring and coaching programmes offered at the various institutions.
- On 8 Mar 2018, the EPFL Alumni and Equality offices organized an event on "Careers for Women... EPFL and beyond" for the International Women's Day. MARVEL had a booth with information about its activities regarding equal opportunities. The event will be renewed on 8 Mar 2019, also with MARVEL participation.

Visibility of women scientists in MARVEL

We make an effort to ensure and increase visibility of women researchers within MARVEL and to recognize their excellence: in year 5, 1 out of 4 distinguished lecturers (Sally Price), 3 out of 14 keynote speakers at COMDI 2018, 5 out of 24 women scientists on the MARVEL booth at Scientastic, 1 out of 6 supervising students for the next summer camp for high school students. They have received several prizes and distinctions: Claire Villevieille, new phase II PI, is a recipient of the SNSF PRIMA grant. Clémence Corminboeuf received an ERC Consolidator Grant and Nicola Spaldin was part of the 4-people team receiving an ERC Synergy Grant (SAB member G. Aeppli also involved). EPFL's Institute of Materials (IMX) now has an installation ($2\ \text{m} \times 2\ \text{m}$, (Fig. 12)) displayed in the Institute's entry hall featuring the 10 women faculty members of the department. The project, sponsored by IMX and MARVEL, was initiated by Nicola Marzari in 2016. It was designed by the graphic designer Alban Kakulya and provides a powerful message to all passing students and researchers.

Work-life balance

- Two SNSF Flexibility grants to help cover the external childcare costs were assigned to MARVEL parents in 2018.
- As mentioned in the strategy, we will prepare a survey to identify good practices already in place in MARVEL labs and existing needs. New measures will be put in place accordingly.

Actions for young girls

- 2 editions of the Polythèmes workshop on materials *Diamant, alu, caoutchouc, ils sont*

fous ces matériaux ! for girls only in Jan and Oct-Nov 2018. Next edition Mar-Apr 2019.

- 4^{th} edition of the summer camp *Matériaux super géniaux* for girls only in Aug 2018.
- Chemistry summer camp for girls and boys (with 50% girls) in Aug 2018.
- Continuation of the support of the mathematic workshops *Maths en jeu*.
- Support to the new project initiated by the EPFL Science Outreach Department with the support of the Federal Office for Gender Equality, the *Coding club des filles*, which offers coding workshops for girls 11 to 15 years old organized throughout French-speaking Switzerland (Fig. 12). These workshops are highly successful and benefit from strong press coverage.

Communication

Internal communication

The MARVEL community received 10 internal newsletters.
Moreover, they have been sent in Jan 2019 a *welcome letter* summarizing what MARVEL is, as well as critical organizational details, including finances, publications acknowledgements, gender-awareness issues and tech transfer. It will be sent to all future MARVEL members.

External communication

Our website saw a 40% increase in users over the calendar year. We added some 20 feature stories and science highlights focused on the research of the group in addition to 37 news stories on awards, conferences and other news of interest to the broader community.
Our Twitter account @nccr_marvel, launched in Nov 2017, now has more than 550 followers and is growing. The most successful Tweets generated engagement rates of more than 11%.
Ten scientific newsletters were sent to an external scientific audience.

Events

For informed audiences

- International Workshop on Computational Design and Discovery of Novel Materials COMDI 2018 (Fig. 11) organized by MARVEL PIs, 10 – 12 Sep 2018, EPFL, including the internal Review and Retreat on 12 Sep 2018.
- 4 distinguished lectures: Prof. Feliciano Giustino (Univ. Oxford), Prof. Sally Price (Univ. College London), Prof. Raffaele Resta (Democritos, Trieste), Prof. Kieron Burke (Univ. California, Irvine).
- 9 MARVEL junior seminars at EPFL.
- Education seminar "Interdisciplinary Learning via Real World Problems: The Agonies and Ecstasies of the UMass iCons Program" by Scott Auerbach (UMass Amherst, USA), 21 Jun 2018.

Figure 13: *Left: ACCES Visualization Contest exhibition, EPFL, Feb-Mar 2018. Right: Ig Nobel Award Tour Show at EPFL, 27 Mar 2018.*

For the public at large

- ACCES Visualization Contest: award ceremony 26 Feb 2018 and exhibition 26 Feb – 21 Mar 2018 at EPFL (Fig. 13).
- Ig Nobel Award Tour Show, 27 Mar 2018 (Fig. 13).
- Unveiling of artwork featuring women scientists at EPFL's Institute of Materials, 8 Nov 2018 (Fig. 12).
- MARVEL booth at EPFL Scientastic, 10 – 11 Nov 2018, with 3D movies and fun experiments to show how novel materials are created by computational design.
- 5 MARVEL PhD students at EPFL participated to the selections of "My Thesis in 180 s" in Jan 2019. We will know soon how many of them are selected for the EPFL finale on 7 Mar 2019.

MARVEL in the news — some highlights

- Thousands of 2D materials are just waiting to be discovered, *Chemistry World*, 15 Feb 2018.
- Nanotechnology treasure trove, *Science Daily*, 6 Mar 2018.
- A treasure trove for nanotechnology experts, *Phys.Org*, 7 Mar 2018.
- How AI is helping us discover materials faster than ever, *The Verge*, 25 Apr 2018.
- Scienza, dalle simulazioni quantistiche i materiali del futuro, *Askanews*, 4 May 2018.
- I miei 2 mila nuovi materiali trasformeranno il mondo, *La Stampa*, 8 May 2018.

2 Reaction to the review panel recommendations

Response to general impressions

We thank the panel for the very positive feedback given to the project, and the care put into evaluating the broader goals, detailed implementation and projects, and structural efforts. Phase I (Building community and tools) has indeed created and nucleated many collaborations both at the computational and at the experimental level, while ramping up the methodological capabilities needed to achieve some of the core goals in computational design and discovery. It has also formulated a long-term vision where the infrastructural platforms leverage and strengthen the entire effort in the unique way that is only possible through a sustained and long-term vision.
Phase II (Design and discovery of novel materials), as formulated in the Full Proposal, takes now the form of targeted projects that involve core groups of theoretical and experimental groups working together. We monitor progress in all these projects, and the Review and Retreat of September 2019 will be a key moment for cross evaluation and adjustment, helped by the counsel of our own Scientific Advisory Board, to allow for a dynamical process where projects grow or decrease in size, and new efforts are ignited.

Response to scientific progress

The report mentions "much progress and many extraordinary results" and that the "excellent quality of the science done in the NCCR MARVEL is indisputable". Without dwelling on the positives, three concerns are mentioned: "that not enough people contribute to the open science platform AiiDA", "the loss of some interesting and promising activities", and that "the methodology part has become quite small".
The first concern is also balanced by the statement "the platforms are very useful to disseminate the data between the different groups of the consortium and beyond" and that "AiiDA and Materials Cloud are clearly taking off now [...] and they are a great service of MARVEL to the international community in computational materials." Most importantly, our recent developments within the MARVEL OSP (Materials Cloud, the web GUIs of the AiiDA Lab, the constant development of robust automated workflows for the simulation of materials properties) are fostering and facilitating the adoption of AiiDA. As an example, in the past $\sim$ 20 months (since the AiiDA plugin registry went online, with less than 5 code plugins), the number of plugins increased to 27 entries supporting 59 different simulation codes (many of which routinely used by MARVEL groups), and over 50 different workflows (Fig. 1). Furthermore, we have been able to engage also communities outside MARVEL, with major project partners (like the H2020 MaX Centre of Excellence (2015-18, 2018-21), H2020 MarketPlace (2018-22), H2020 INTERSECT (2019-21), swissuniversities P5 "Materials Cloud" and OSSCAR of the EPFL Open Science fund), in addition to many contributions by independent researchers.

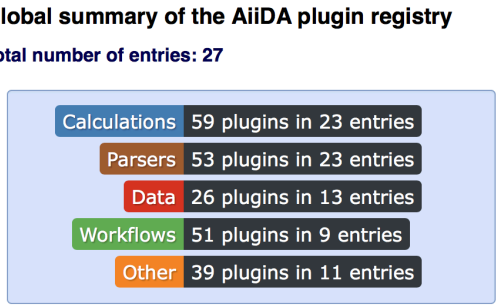

Figure 1: *AiiDA plugin registry statistics. Almost 60 external simulation codes are now supported, with over 50 different workflows implemented.*

The second comment is taken at heart, but is ultimately the result of having finite resources, and the need to have a dynamics that rewards the projects that are more successful, collaborative, and integrated in the goals and metrics of the entire effort.
The last comment reflects the request we had in the June 2016 SNSF report to focus on collaborative grand challenges, where multidisci-

plinary teams work on the same problem, with a significant experimental component — until then, the NCCR was structured to nurture also independent methodological efforts, and that has been the case for the entire duration of phase I. It should also be mentioned that the Swiss ecosystem is particularly supportive of methodological efforts, thanks to the substantial support coming from SNSF individual projects, University chairs, the Platform for Advanced Scientific Computing (PASC), complemented by the EU ERC grants. Proposal for fully methodological projects that fulfill the SNSF and MARVEL goals of being open-source, collaborative, long-term, and structural would also be very welcome.

Response to management-related areas

For Knowledge and technology transfer, we underscore how our international visibility is starting to attract considerable industrial engagement and funding, with major companies drafting MARVEL-wide agreements. For Education and training, the only uphill challenge will indeed be the establishment of an advanced training programme, given the difficulty of offering classes cutting across Departments and Faculties. For Equal opportunities, we truly sympathize with the panel's comments, and a dedicated and extensive response is offered in Annex 2. For Communication, the hiring of Carey Sargent and the engagement of Fiorien Bonthuis has provided an excellent stream of scientific highlights, feature stories, and a Twitter audience that has already reached more than 550 users.

Response to final recommendations

The three final recommendations concern the integration of machine learning and methodology expertise, the equal opportunity efforts, and the industrial engagement.
For the first one, machine learning not only has its own dedicated project, but is very much integrated into many projects, especially D&D1, D&D2, D&D4 and D&D6 and Inc1. For the second one, as mentioned we provide a dedicated and extensive response in Annex 2. For the last recommendation, we believe that the creation of an Industrial Advisory Board, the ongoing Sector Days, the contractual engagement of major industries, and the leading role played by William Curtin in driving these activities together with Pascale van Landuyt, as well as Daniele Passerone at Empa, are positioning us very favorably for the next years.

3 Changes in PIs

No changes in PIs since the Full Proposal for phase II.

4 Structural Developments

No structural development to report at this stage.

Annex 1 Publication list

All publications have been entered in NIRA, and are listed below, sorted by group leaders. The following lists cover the period from February 1st, 2018 to January 31st, 2019.

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

Phase II PIs

Group of Ulrich Aschauer

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

M. Porer, M. Fechner, E. M. Bothschafter, L. Rettig, M. Savoini, V. Esposito, J. Rittmann, M. Kubli, M. J. Neugebauer, E. Abreu, T. Kubacka, T. Huber, G. Lantz, S. Parchenko, S. Grübel, A. Paarmann, J. Noack, P. Beaud, G. Ingold, U. Aschauer, S. L. Johnson, and U. Staub
Ultrafast Relaxation Dynamics of the Antiferrodistortive Phase in Ca Doped $SrTiO_3$
Physical Review Letters **121**, 055701 (2018).
Group(s): Aschauer, Staub / Project(s): PP7, DD5

Group of Michele Ceriotti

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

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

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

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

F. M. Paruzzo, A. Hofstetter, F. Musil, S. De, M. Ceriotti, and L. Emsley
Chemical shifts in molecular solids by machine learning
Nature Communications **9**, 4501 (2018).
Group(s): Ceriotti / Project(s): DD1

M. J. Willatt, F. Musil, and M. Ceriotti
Feature Optimization for Atomistic Machine Learning Yields a Data-Driven Construction of the Periodic Table of the Elements
Physical Chemistry Chemical Physics **20**, 29661 (2018).
Group(s): Ceriotti / Project(s): DD1, DD2

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

A. Cuzzocrea, R. H. Meissner, D. M. Wilkins, B. A. Helfrecht, P. Juda, S. P. Bienvenue, W. Fang, J. Kessler, I. Poltavsky, S. Vandenbrande, J. Wieme, C. Corminboeuf, T. D. Kühne, D. E. Manolopoulos, T. E. Markland, J. O. Richardson, A. Tkatchenko, G. A. Tribello, V. V. Speybroeck, and M. Ceriotti
i-PI 2.0: A universal force engine for advanced molecular simulations
Computer Physics Communications (2018), doi:10.1016/j.cpc.2018.09.020.
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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

A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti
Transferable Machine-Learning Model of the Electron Density
ACS Central Science **5**, 57 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

Group of Clémence Corminboeuf

V. Kapil, M. Rossi, O. Marsalek, R. Petraglia, Y. Litman, T. Spura, B. Cheng, A. Cuzzocrea, R. H. Meissner, D. M. Wilkins, B. A. Helfrecht, P. Juda, S. P. Bienvenue, W. Fang, J. Kessler, I. Poltavsky, S. Vandenbrande, J. Wieme, C. Corminboeuf, T. D. Kühne, D. E. Manolopoulos, T. E. Markland, J. O. Richardson, A. Tkatchenko, G. A. Tribello, V. V. Speybroeck, and M. Ceriotti
i-PI 2.0: A universal force engine for advanced molecular simulations
Computer Physics Communications (2018), doi:10.1016/j.cpc.2018.09.020.
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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

A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti
Transferable Machine-Learning Model of the Electron Density
ACS Central Science **5**, 57 (2019).
Group(s): Ceriotti, Corminboeuf / Project(s): DD1

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

M. Busch, M. D. Wodrich, and C. Corminboeuf
Improving the Thermodynamic Profiles of Prospective Suzuki-Miyaura Cross-Coupling Catalysts by Altering the Electrophilic Coupling Component
ChemCatChem **10**, 1592 (2018).
Group(s): Corminboeuf / Project(s): VP2

M. D. Wodrich, B. Sawatlon, M. Busch, and C. Corminboeuf
On the Generality of Molecular Volcano Plots
ChemCatChem **10**, 1586 (2018).
Group(s): Corminboeuf / Project(s): VP2

M. D. Wodrich, M. Busch, and C. Corminboeuf
Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction
Helvetica Physica Acta **101**, e1800107 (2018).
Group(s): Corminboeuf / Project(s): VP2

M. Busch, A. Fabrizio, S. Luber, J. Hutter, and C. Corminboeuf
Exploring the Limitation of Molecular Water Oxidation Catalysts
The Journal of Physical Chemistry C **122**, 12404 (2018).
Group(s): Corminboeuf, Hutter / Project(s): VP2

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

Group of William Curtin

B. Yin and W. A. Curtin
First-principles-based prediction of yield strength in the RhIrPdPtNiCu high entropy alloy
npj Computational Materials **5**, 14 (2019).
Group(s): Curtin / Project(s): DD2

P. Andric, B. Yin, and W. A. Curtin
Stress-dependence of generalized stacking fault energies
Journal of the Mechanics and Physics of Solids **122**, 262 (2019).
Group(s): Curtin / Project(s): DD2

F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin
Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential
npj Computational Materials **4**, 69 (2018).
Group(s): Curtin, Marzari / Project(s): DD2

Group of Claude Ederer

S. Beck, G. Sclauzero, U. Chopra, and C. Ederer
Metal-insulator transition in $CaVO_3$ thin films: Interplay between epitaxial strain, dimensional confinement, and surface effects
Physical Review B **97**, 075107 (2018).
Group(s): Ederer / Project(s): DD5

D. E. McNally, X. Lu, J. Pelliciari, S. Beck, M. Dantz, M. Naamneh, T. Shang, M. Medarde, C. W. Schneider, V. N. Strocov, E. V. Pomjakushina, C. Ederer, M. Radovic, and T. Schmitt
Electronic localization in $CaVO_3$ films via bandwidth control
npj Quantum Materials **4**, 6 (2019).
Group(s): Ederer, Medarde, Schmitt / Project(s): PP7

Group of Roman Fasel

O. Gröning, S. Wang, X. Yao, C. A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Müllen, P. Ruffieux, and R. Fasel
Engineering of robust topological quantum phases in graphene nanoribbons
Nature **560**, 209 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

S. Mishra, M. Krzeszewski, C. A. Pignedoli, P. Ruffieux, R. Fasel, and D. T. Gryko
On-surface synthesis of a nitrogen-embedded buckybowl with inverse Stone-Thrower-Wales topology
Nature Communications **9**, 1714 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

S. Mishra, T. G. Lohr, C. A. Pignedoli, J. Liu, R. Berger, J. I. Urgel, K. Müllen, X. Feng, P. Ruffieux, and R. Fasel
Tailoring Bond Topologies in Open-Shell Graphene Nanostructures
ACS Nano **12**, 11917 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

X.-Y. Wang, J. I. Urgel, G. B. Barin, K. Eimre, M. Di Giovannantonio, A. Milani, M. Tommasini, C. A. Pignedoli, P. Ruffieux, X. Feng, R. Fasel, K. Müllen, and A. Narita
Bottom-Up Synthesis of Heteroatom-Doped Chiral Graphene Nanoribbons
Journal of the American Chemical Society **140**, 9104 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

A. V. Yakutovich, J. Hoja, D. Passerone, A. Tkatchenko, and C. A. Pignedoli
Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111)
Journal of the American Chemical Society **140**, 1401 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

M. Di Giovannantonio, J. I. Urgel, U. Beser, A. V. Yakutovich, J. Wilhelm, C. A. Pignedoli, P. Ruffieux, A. Narita, K. Müllen, and R. Fasel
On-Surface Synthesis of Indenofluorene Polymers by Oxidative Five-Membered Ring Formation
Journal of the American Chemical Society **140**, 3532 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

Group of Stefan Goedecker

M. Graužinytė, S. Goedecker, and J. A. Flores-Livas
Towards bipolar tin monoxide: Revealing unexplored dopants
Physical Review Materials **2**, 104604 (2018).
Group(s): Goedecker / Project(s): DD1

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

D. S. De, S. Saha, L. Genovese, and S. Goedecker

Influence of an external electric field on the potential-energy surface of alkali-metal-decorated C_{60}

Physical Review A **97**, 063401 (2018).

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

L. E. Ratcliff, A. Degomme, J. A. Flores-Livas, S. Goedecker, and L. Genovese

Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers

Journal of Physics: Condensed Matter **30**, 095901 (2018).

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

J. S. C. Kearney, M. Graužinytė, D. Smith, D. Sneed, C. Childs, J. Hinton, C. Park, J. S. Smith, E. Kim, S. D. S. Fitch, A. L. Hector, C. J. Pickard, J. A. Flores-Livas, and A. Salamat

Pressure-Tuneable Visible-Range Band Gap in the Ionic Spinel Tin Nitride

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

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

J. A. Flores-Livas, M. Graužinytė, L. Boeri, G. Profeta, and A. Sanna

Superconductivity in doped polyethylene at high pressure

The European Physical Journal B **91**, 176 (2018).

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

O. Andreussi and G. Fisicaro

Continuum embeddings in condensed-matter simulations

International Journal of Quantum Chemistry **119**, e25725 (2018).

Group(s): Goedecker, Marzari / Project(s): Inc1

J. A. Flores-Livas, D. Tomerini, M. Amsler, A. Boziki, U. Rothlisberger, and S. Goedecker

Emergence of hidden phases of methylammonium lead iodide ($CH_3NH_3PbI_3$) upon compression

Physical Review Materials **2**, 085201 (2018).

Group(s): Goedecker, Röthlisberger / Project(s): DD1, VP2, HP4

Group of Jürg Hutter

M. Busch, A. Fabrizio, S. Luber, J. Hutter, and C. Corminboeuf

Exploring the Limitation of Molecular Water Oxidation Catalysts

The Journal of Physical Chemistry C **122**, 12404 (2018).

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

T. Musso, S. Caravati, J. Hutter, and M. Iannuzzi

Second generation Car-Parrinello MD: application to the h-BN/Rh(111) nanomesh

The European Physical Journal B **91**, 148 (2018).

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

D. Golze, J. Wilhelm, M. J. van Setten, and P. Rinke

Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis

Journal of Chemical Theory and Computation **14**, 4856 (2018).

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

Group of Mathieu Luisier

N. Cavassilas, D. Logoteta, Y. Lee, F. Michelini, M. Lannoo, M. Bescond, and M. Luisier

Dual-Gated $WTe_2/MoSe_2$ van der Waals Tandem Solar Cell

The Journal of Physical Chemistry C **122**, 28545 (2018).

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

C. Klinkert, A. Szabo, D. Campi, C. Stieger, N. Marzari, and M. Luisier

Novel 2-D Materials for Tunneling FETs: an Ab-initio Study

in *2018 76th Device Research Conference (DRC)* (IEEE, 2018), pp. 1–2.

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

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

Ab Initio Simulation of Band-to-Band Tunneling FETs With Single- and Few-Layer 2-D Materials as Channels

IEEE Transactions on Electron Devices **65**, 4180 (2018).

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

Group of Nicola Marzari

J. Huang, N. Hörmann, E. Oveisi, A. Loiudice, G. L. De Gregorio, O. Andreussi, N. Marzari, and R. Buonsanti

Potential-induced nanoclustering of metallic catalysts during electrochemical CO_2 reduction

Nature Communications **9**, 3117 (2018).

Group(s): Buonsanti, Marzari / Project(s): PP7, Inc1

F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin

Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential

npj Computational Materials **4**, 69 (2018).

Group(s): Curtin, Marzari / Project(s): DD2

O. Andreussi and G. Fisicaro

Continuum embeddings in condensed-matter simulations

International Journal of Quantum Chemistry **119**, e25725 (2018).

Group(s): Goedecker, Marzari / Project(s): Inc1

C. Klinkert, A. Szabo, D. Campi, C. Stieger, N. Marzari, and M. Luisier

Novel 2-D Materials for Tunneling FETs: an Ab-initio Study

in *2018 76th Device Research Conference (DRC)* (IEEE, 2018), pp. 1–2.

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

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

Ab Initio Simulation of Band-to-Band Tunneling FETs With Single- and Few-Layer 2-D Materials as Channels

IEEE Transactions on Electron Devices **65**, 4180 (2018).

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

K. Alberi, M. B. Nardelli, A. Zakutayev, L. Mitas, S. Curtarolo, A. Jain, M. Fornari, N. Marzari, I. Takeuchi, M. L. Green, M. Kanatzidis, M. F. Toney, S. Butenko, B. Meredig, S. Lany, U. Kattner, A. Davydov, E. S. Toberer, V. Stevanovic, A. Walsh, N.-G. Park, A. Aspuru-Guzik, D. P. Tabor, J. Nelson, J. Murphy, A. Setlur, J. Gregoire, H. Li, R. Xiao, A. Ludwig, L. W. Martin, A. M. Rappe, S.-H. Wei, and J. Perkins

The 2019 materials by design roadmap

Journal of Physics D: Applied Physics **52**, 013001 (2019).

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

A. Marrazzo, M. Gibertini, D. Campi, N. Mounet, and N. Marzari

Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator

Physical Review Letters **120**, 117701 (2018).

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

N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi, and N. Marzari

Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds

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

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

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

Precision and efficiency in solid-state pseudopotential calculations

npj Computational Materials **4**, 72 (2018).

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

T. Sohier, D. Campi, N. Marzari, and M. Gibertini

Mobility of two-dimensional materials from first principles in an accurate and automated framework

Physical Review Materials **2**, 114010 (2018).

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

N. Colonna, N. L. Nguyen, A. Ferretti, and N. Marzari

Screening in Orbital-Density-Dependent Functionals

Journal of Chemical Theory and Computation **14**, 2549 (2018).

Group(s): Marzari / Project(s): HP3

N. G. Hörmann, O. Andreussi, and N. Marzari

Grand canonical simulations of electrochemical interfaces in implicit solvation models

The Journal of Chemical Physics **150**, 041730 (2019).

Group(s): Marzari / Project(s): Inc1

L. Kahle, A. Marcolongo, and N. Marzari

Modeling lithium-ion solid-state electrolytes with a pinball model

Physical Review Materials **2**, 065405 (2018).

Group(s): Marzari / Project(s): Inc1

F. Nattino, M. Truscott, N. Marzari, and O. Andreussi

Continuum models of the electrochemical diffuse layer in electronic-structure calculations

The Journal of Chemical Physics **150**, 041722 (2019).

Group(s): Marzari / Project(s): Inc1

N. L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari

Koopmans-Compliant Spectral Functionals for Extended Systems

Physical Review X **8**, 021051 (2018).

Group(s): Marzari / Project(s): HP3

I. Timrov, N. Marzari, and M. Cococcioni

Hubbard parameters from density-functional perturbation theory

Physical Review B **98**, 085127 (2018).

Group(s): Marzari / Project(s): Inc1

B.-J. Kim, X. Cheng, D. F. Abbott, E. Fabbri, F. Bozza, T. Graule, I. E. Castelli, L. Wiles, N. Danilovic, K. E. Ayers, N. Marzari, and T. J. Schmidt

Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+\delta}$ and $PrBaCo_2O_{5+\delta}$

Advanced Functional Materials **28**, 1804355 (2018).

Group(s): Marzari, Schmidt / Project(s): PP7, Inc1

Group of Marisa Medarde

D. E. McNally, X. Lu, J. Pelliciari, S. Beck, M. Dantz, M. Naamneh, T. Shang, M. Medarde, C. W. Schneider, V. N. Strocov, E. V. Pomjakushina, C. Ederer, M. Radovic, and T. Schmitt

Electronic localization in $CaVO_3$ films via bandwidth control

npj Quantum Materials **4**, 6 (2019).

Group(s): Ederer, Medarde, Schmitt / Project(s): PP7

D. J. Gawryluk, J. Rodríguez-Carvajal, P. Lacorre, M. T. Fernández-Díaz, and M. Medarde

Distortion mode anomalies in bulk $PrNiO_3$

arXiv:1809.10914 (2018).

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

Group of Michele Parrinello

P. M. Piaggi and M. Parrinello

Predicting polymorphism in molecular crystals using orientational entropy

Proceedings of the National Academy of Science of the USA **115**, 10251 (2018).

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

D. Mendels, J. McCarty, P. M. Piaggi, and M. Parrinello

Searching for Entropically Stabilized Phases: The Case of Silver Iodide

The Journal of Physical Chemistry C **122**, 1786 (2018).

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

K. Tarak, P. M. Piaggi, C. Perego, and M. Parrinello

A Cannibalistic Approach to Grand Canonical Crystal Growth

Journal of Chemical Theory and Computation **14**, 2678 (2018).

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

H. Niu, P. M. Piaggi, M. Invernizzi, and M. Parrinello

Molecular dynamics simulations of liquid silica crystallisation

Proceedings of the National Academy of Science of the USA **115**, 5348 (2018).

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

Y. Wang, O. Valsson, P. Tiwary, M. Parrinello, and K. Lindorff-Larsen

Frequency adaptive metadynamics for the calculation of rare-event kinetics

The Journal of Chemical Physics **149**, 072309 (2018).

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

C. Perego, O. Valsson, and M. Parrinello

Chemical potential calculations in non-homogeneous liquids

The Journal of Chemical Physics **149**, 072305 (2018).

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

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

Combining Metadynamics and Integrated Tempering Sampling

The Journal of Physical Chemistry Letters **9**, 6426 (2018).

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

L. Bonati and M. Parrinello

Silicon liquid structure and crystal nucleation from ab initio *deep metadynamics*

Physical Review Letters **121**, 265701 (2018).

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

P. M. Piaggi and M. Parrinello

Multithermal-multibaric molecular simulations from a variational principle

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

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

D. Han, T. Karmakar, Z. Bjelobrk, J. Gong, and M. Parrinello

Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies

Chemical Engineering Science (2018), doi:10.1016/j.ces.2018.10.022.

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

Y. I. Yang and M. Parrinello

Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling

Journal of Chemical Theory and Computation

14, 2889 (2018).
Group(s): Parrinello / Project(s): DD1

Group of Alfredo Pasquarello

J. Wiktor, I. Reshetnyak, M. Strach, M. Scarongella, R. Buonsanti, and A. Pasquarello
Sizable excitonic effects undermining the photocatalytic efficiency of β-$Cu_2V_2O_7$
The Journal of Physical Chemistry Letters **9**, 5698 (2018).
Group(s): Buonsanti, Pasquarello / Project(s): VP2, PP7, DD4

A. Bouzid and A. Pasquarello
Atomic-scale simulation of electrochemical processes at electrode/water interfaces under referenced bias potential
The Journal of Physical Chemistry Letters **9**, 1880 (2018).
Group(s): Pasquarello / Project(s): VP2, DD3, DD4

P. Gono, J. Wiktor, F. Ambrosio, and A. Pasquarello
Surface polarons reducing overpotentials of the oxygen evolution reaction
ACS Catalysis **8**, 5847 (2018).
Group(s): Pasquarello / Project(s): VP2, DD3, DD4

P. Oberholzer, E. Tervoort, A. Bouzid, A. Pasquarello, and D. Kundu
Oxide versus Nonoxide Cathode Materials for Aqueous Zn Batteries: An Insight into the Charge Storage Mechanism and Consequences Thereof
ACS Applied Materials & Interfaces **11**, 674 (2019).
Group(s): Pasquarello / Project(s): VP2, DD3, DD4

Z. Guo, F. Ambrosio, and A. Pasquarello
Extrinsic defects in amorphous oxides: Hydrogen, carbon, and nitrogen impurities in alumina
to be published in Physical Review Applied (2019).
Group(s): Pasquarello / Project(s): DD3, DD4

F. Ambrosio, J. Wiktor, and A. Pasquarello
pH-dependent catalytic reaction pathway for water splitting at the $BiVO_4$-water interface from the band alignment
ACS Energy Letters **3**, 829 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

F. Ambrosio, J. Wiktor, and A. Pasquarello
pH-dependent surface chemistry from first principles: Application to the $BiVO_4$(010)-water interface
ACS Applied Materials & Interfaces **10**, 10011 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

F. Ambrosio, Z. Guo, and A. Pasquarello
Absolute energy levels of liquid water
The Journal of Physical Chemistry Letters **9**, 3212 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

Z. Guo, F. Ambrosio, and A. Pasquarello
Hole diffusion across leaky amorphous TiO_2 coating layers for catalytic water splitting at photoanodes
Journal of Materials Chemistry A **6**, 11804 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

J. Wiktor, F. Ambrosio, and A. Pasquarello
Role of polarons in water splitting: The case of $BiVO_4$
ACS Energy Letters **3**, 1693 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

J. Wiktor, F. Ambrosio, and A. Pasquarello
Mechanism suppressing charge recombination at iodine defects in $CH_3NH_3PbI_3$ by polaron formation
Journal of Materials Chemistry A **6**, 16863 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

F. Ambrosio and A. Pasquarello
Reactivity and energy level of a localized hole in liquid water
Physical Chemistry Chemical Physics **20**, 30281 (2018).
Group(s): Pasquarello / Project(s): VP2, DD4

Group of Daniele Passerone

O. Gröning, S. Wang, X. Yao, C. A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Müllen, P. Ruffieux, and R. Fasel
Engineering of robust topological quantum phases in graphene nanoribbons
Nature **560**, 209 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

S. Mishra, M. Krzeszewski, C. A. Pignedoli, P. Ruffieux, R. Fasel, and D. T. Gryko

On-surface synthesis of a nitrogen-embedded buckybowl with inverse Stone-Thrower-Wales topology

Nature Communications **9**, 1714 (2018).

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

S. Mishra, T. G. Lohr, C. A. Pignedoli, J. Liu, R. Berger, J. I. Urgel, K. Müllen, X. Feng, P. Ruffieux, and R. Fasel

Tailoring Bond Topologies in Open-Shell Graphene Nanostructures

ACS Nano **12**, 11917 (2018).

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

X.-Y. Wang, J. I. Urgel, G. B. Barin, K. Eimre, M. Di Giovannantonio, A. Milani, M. Tommasini, C. A. Pignedoli, P. Ruffieux, X. Feng, R. Fasel, K. Müllen, and A. Narita

Bottom-Up Synthesis of Heteroatom-Doped Chiral Graphene Nanoribbons

Journal of the American Chemical Society **140**, 9104 (2018).

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

A. V. Yakutovich, J. Hoja, D. Passerone, A. Tkatchenko, and C. A. Pignedoli

Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111)

Journal of the American Chemical Society **140**, 1401 (2018).

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

M. Di Giovannantonio, J. I. Urgel, U. Beser, A. V. Yakutovich, J. Wilhelm, C. A. Pignedoli, P. Ruffieux, A. Narita, K. Müllen, and R. Fasel

On-Surface Synthesis of Indenofluorene Polymers by Oxidative Five-Membered Ring Formation

Journal of the American Chemical Society **140**, 3532 (2018).

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

Group of Daniele Pergolesi

D. Pergolesi, E. Gilardi, E. Fabbri, V. Roddatis, G. F. Harrington, T. Lippert, J. A. Kilner, and E. Traversa

Interface Effects on the Ionic Conductivity of Doped Ceria–Yttria-Stabilized Zirconia Heterostructures

ACS Applied Materials & Interfaces **10**, 14160 (2018).

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

F. Haydous, W. Si, V. A. Guzenko, F. Waag, E. Pomjakushina, M. El Kazzi, L. Sévery, A. Wokaun, D. Pergolesi, and T. Lippert

Improved Photoelectrochemical Water Splitting of $CaNbO_2N$ Photoanodes by CoPi Photodeposition and Surface Passivation

The Journal of Physical Chemistry C **123**, 1059 (2019).

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

Group of Giovanni Pizzi

T. Gorni, I. Timrov, and S. Baroni

Spin dynamics from time-dependent density functional perturbation theory

The European Physical Journal B **91**, 249 (2018).

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

R. Mercado, R.-S. Fu, A. V. Yakutovich, L. Talirz, M. Haranczyk, and B. Smit

In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications

Chemistry of Materials **30**, 5069 (2018).

Group(s): Smit, Pizzi / Project(s): DD4, OSP

Group of Volker Roth

A. Kortylewski, M. Wieser, A. Morel-Forster, A. Wieczore, S. Parbhoo, V. Roth, and T. Vetter

Informed MCMC with Bayesian Neural Networks for Facial Image Analysis

in *NeurIPS 2018 Workshop on Bayesian Deep Learning* (Montreal, 2018).

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

S. Parbhoo, M. Wieser, and V. Roth

Cause-Effect Deep Information Bottleneck for Incomplete Covariates

in *NeurIPS 2018 Workshop on Causal Learning* (Montreal, 2018).

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

S. Parbhoo, M. Wieser, and V. Roth

Estimating Causal Effects With Partial Covariates For Clinical Interpretability

in *NeurIPS 2018 Workshop on Machine Learning for Health* (Montreal, 2018).

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

Group of Ming Shi

N. Xu, Z. W. Wang, A. Magrez, P. Bugnon, H. Berger, C. E. Matt, V. N. Strocov, N. C. Plumb, M. Radovic, E. Pomjakushina, K. Conder, J. H. Dil, J. Mesot, R. Yu, H. Ding, and M. Shi

Evidence of Coulomb-interaction-induced Lifshitz transition and robust hybrid Weyl semimetal in T_d-$MoTe_2$

Physical Review Letters **121**, 136401 (2018).

Group(s): Shi / Project(s): PP7, DD6

A. P. Weber, P. Rüssmann, N. Xu, S. Muff, M. Fanciulli, A. Magrez, P. Bugnon, H. Berger, N. C. Plumb, M. Shi, S. Blügel, P. Mavropoulos, and J. H. Dil

Spin-resolved electronic response to the phase transition in $MoTe_2$

Physical Review Letters **121**, 156401 (2018).

Group(s): Shi / Project(s): PP7, DD6

C.-J. Yi, B. Q. Lv, Q. S. Wu, B.-B. Fu, X. Gao, M. Yang, X.-L. Peng, M. Li, Y.-B. Huang, P. Richard, M. Shi, G. Li, O. V. Yazyev, Y.-G. Shi, T. Qian, and H. Ding

Observation of a nodal chain with Dirac surface states in TiB_2

Physical Review B **97**, 201107(R) (2018).

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

N. Xu, Y. T. Qian, Q. S. Wu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, V. N. Strocov, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, O. V. Yazyev, T. Qian, H. Ding, J. Mesot, and M. Shi

Trivial topological phase of CaAgP and the topological nodal-line transition in $CaAg(P_{1-x}As_x)$

Physical Review B **97**, 161111(R) (2018).

Group(s): Shi, Yazyev / Project(s): PP7, DD6

Group of Berend Smit

S. Barthel, E. V. Alexandrov, D. M. Proserpio, and B. Smit

Distinguishing Metal–Organic Frameworks

Crystal Growth & Design **18**, 1738 (2018).

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

E. Braun, Y. Lee, S. M. Moosavi, S. Barthel, R. Mercado, I. A. Baburin, D. M. Proserpio, and B. Smit

Generating carbon schwarzites via zeolite-templating

Proceedings of the National Academy of Science of the USA **115**, E8116 (2018).

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

Y. Lee, S. D. Barthel, P. Dłotko, S. M. Moosavi, K. Hess, and B. Smit

High-Throughput Screening Approach for Nanoporous Materials Genome Using Topological Data Analysis: Application to Zeolites

Journal of Chemical Theory and Computation **14**, 4427 (2018).

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

S. M. Moosavi, P. G. Boyd, L. Sarkisov, and B. Smit

Improving the Mechanical Stability of Metal–Organic Frameworks Using Chemical Caryatids

ACS Central Science **4**, 832 (2018).

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

D. Ongari, P. G. Boyd, O. Kadioglu, A. K. Mace, S. Keskin, and B. Smit

Evaluating charge equilibration methods to generate electrostatic fields in nanoporous materials

Journal of Chemical Theory and Computation **15**, 382 (2019).

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

M. Witman, S. Ling, P. Boyd, S. Barthel, M. Haranczyk, B. Slater, and B. Smit

Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of 2D Zeolites

ACS Central Science **4**, 235 (2018).

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

R. Mercado, R.-S. Fu, A. V. Yakutovich, L. Talirz, M. Haranczyk, and B. Smit

In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications

Chemistry of Materials **30**, 5069 (2018).

Group(s): Smit, Pizzi / Project(s): DD4, OSP

S. Kampouri, T. N. Nguyen, C. P. Ireland, B. Valizadeh, F. M. Ebrahim, G. Capano, D. Ongari, A. Mace, N. Guijarro, K. Sivula, A. Sienkiewicz, L. Forró, B. Smit, and K. C. Stylianou

Photocatalytic hydrogen generation from a visible-light responsive metal-organic framework system: the impact of nickel phosphide nanoparticles

Journal of Materials Chemistry A **6**, 2476 (2018).

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

T. N. Nguyen, S. Kampouri, B. Valizadeh, W. Luo, D. Ongari, O. M. Planes, A. Züttel, B. Smit, and K. C. Stylianou

Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metal–Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts

ACS Applied Materials & Interfaces **10**, 30035 (2018).

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

S. Kampouri, T. N. Nguyen, M. Spodaryk, R. G. Palgrave, A. Züttel, B. Smit, and

K. C. Stylianou
Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH_2 under Visible Light Irradiation
Advanced Functional Materials **28**, 1806368 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

S. M. Moosavi, A. Chidambaram, L. Talirz, M. Haranczyk, K. C. Stylianou, and B. Smit
Capturing chemical intuition in synthesis of metal-organic frameworks
Nature Communications **10**, 539 (2019).
Group(s): Smit, Stylianou / Project(s): DD4

Group of Alexey Soluyanov

D. Gresch, Q. Wu, G. W. Winkler, R. Häuselmann, M. Troyer, and A. A. Soluyanov
Automated construction of symmetrized Wannier-like tight-binding models from ab initio calculations
Physical Review Materials **2**, 103805 (2018).
Group(s): Soluyanov / Project(s): DD6

S. Singh, Q. Wu, C. Yue, A. H. Romero, and A. A. Soluyanov
Topological phonons and thermoelectricity in triple-point metals
Physical Review Materials **2**, 114204 (2018).
Group(s): Soluyanov / Project(s): VP1, DD6

D. Gresch and A. A. Soluyanov
Calculating topological invariants with Z2Pack
in *Topological Matter. Springer Series in Solid-State Sciences, Vol. 190*, D. Bercioux, J. Cayssol, M. Vergniory, and M. Reyes Calvo, eds. (Springer, Cham, 2018), p. 63.
Group(s): Soluyanov / Project(s): VP1, DD6

Group of Nicola Spaldin

N. S. Fedorova, Y. W. Windsor, C. Findler, M. Ramakrishnan, A. Bortis, L. Rettig, K. Shimamoto, E. M. Bothschafter, M. Porer, V. Esposito, Y. Hu, A. Alberca, T. Lippert, C. W. Schneider, U. Staub, and N. A. Spaldin
Relationship between crystal structure and multiferroic orders in orthorhombic perovskite manganites
Physical Review Materials **2**, 104414 (2018).
Group(s): Spaldin, Staub / Project(s): PP7, VP1, DD5

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

Group of Kyriakos Stylianou

S. Kampouri, T. N. Nguyen, C. P. Ireland, B. Valizadeh, F. M. Ebrahim, G. Capano, D. Ongari, A. Mace, N. Guijarro, K. Sivula, A. Sienkiewicz, L. Forró, B. Smit, and K. C. Stylianou
Photocatalytic hydrogen generation from a visible-light responsive metal-organic framework system: the impact of nickel phosphide nanoparticles
Journal of Materials Chemistry A **6**, 2476 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

T. N. Nguyen, S. Kampouri, B. Valizadeh, W. Luo, D. Ongari, O. M. Planes, A. Züttel, B. Smit, and K. C. Stylianou
Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metal–Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts
ACS Applied Materials & Interfaces **10**, 30035 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

S. Kampouri, T. N. Nguyen, M. Spodaryk, R. G. Palgrave, A. Züttel, B. Smit, and K. C. Stylianou
Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH_2 under Visible Light Irradiation
Advanced Functional Materials **28**, 1806368 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

S. M. Moosavi, A. Chidambaram, L. Talirz, M. Haranczyk, K. C. Stylianou, and B. Smit
Capturing chemical intuition in synthesis of metal-organic frameworks
Nature Communications **10**, 539 (2019).
Group(s): Smit, Stylianou / Project(s): DD4

T. N. Nguyen, F. M. Ebrahim, and K. C. Stylianou
Photoluminescent, upconversion luminescent and nonlinear optical metal-organic frameworks: From fundamental photophysics to potential applications
Coordination Chemistry Reviews **377**, 259 (2018).
Group(s): Stylianou / Project(s): DD4

F. M. Ebrahim, T. N. Nguyen, S. Shyshkanov, A. Gładysiak, P. Favre, A. Zacharia, G. Itskos, P. J. Dyson, and K. C. Stylianou
Selective, Fast-Response, and Regenerable Metal–Organic Framework for Sampling Excess Fluoride Levels in Drinking Water
Journal of the American Chemical Society (2019), doi:10.1021/jacs.8b11907.
Group(s): Stylianou / Project(s): DD4

A. Gładysiak, T. N. Nguyen, M. Spodaryk, J.-H. Lee, J. B. Neaton, A. Züttel, and K. C. Stylianou
Incarceration of Iodine in a Pyrene-Based Metal–Organic Framework
Chemistry–A European Journal **25**, 501 (2019).
Group(s): Stylianou / Project(s): DD4

Group of Anatole von Lilienfeld

F. A. Faber, A. S. Christensen, B. Huang, and O. A. von Lilienfeld
Alchemical and structural distribution based representation for universal quantum machine learning
The Journal of Chemical Physics **148**, 241717 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

A. S. Christensen, F. A. Faber, and O. A. von Lilienfeld
Operators in quantum machine learning: Response properties in chemical space
The Journal of Chemical Physics **150**, 064105 (2019).
Group(s): von Lilienfeld / Project(s): Inc2

S. Fias, K. Y. S. Chang, and O. A. von Lilienfeld
Alchemical Normal Modes Unify Chemical Space
The Journal of Physical Chemistry Letters **10**, 30 (2019).
Group(s): von Lilienfeld / Project(s): Inc2

P. Zaspel, B. Huang, H. Harbrecht, and O. A. von Lilienfeld
Boosting quantum machine learning models with a multilevel combination technique: Pople diagrams revisited
Journal of Chemical Theory and Computation (2018), doi:10.1021/acs.jctc.8b00832.
Group(s): von Lilienfeld / Project(s): Inc2

K. Y. S. Chang and O. A. von Lilienfeld
$Al_xGa_{1-x}As$ crystals with direct 2 eV band gaps from computational alchemy
Physical Review Materials **2**, 073802 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

M. Rupp, O. A. von Lilienfeld, and K. Burke
Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry
The Journal of Chemical Physics **148**, 241401 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

T. Bereau, R. A. DiStasio Jr., A. Tkatchenko, and O. A. von Lilienfeld
Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning
The Journal of Chemical Physics **148**, 241706 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

O. A. von Lilienfeld
Quantum Machine Learning in Chemical Compound Space
Angewandte Chemie International Edition **57**, 4164 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

J. J. Kranz, M. Kubillus, R. Ramakrishnan, O. A. von Lilienfeld, and M. Elstner
Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning
Journal of Chemical Theory and Computation **14**, 2341 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

D. N. Tahchieva, D. Bakowies, R. Ramakrishnan, and O. A. von Lilienfeld
Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations
Journal of Chemical Theory and Computation **14**, 4806 (2018).
Group(s): von Lilienfeld / Project(s): Inc2

Group of Philipp Werner

M. Schüler, M. Eckstein, and P. Werner
Truncating the memory time in nonequilibrium dynamical mean field theory calculations
Physical Review B **97**, 245129 (2018).
Group(s): Werner / Project(s): DD5

Y. Murakami and P. Werner
Nonequilibrium steady states of electric field driven Mott insulators

Physical Review B **98**, 075102 (2018).
Group(s): Werner / Project(s): DD5

P. Werner, H. U. R. Strand, S. Hoshino, Y. Murakami, and M. Eckstein
Enhanced pairing susceptibility in a photodoped two-orbital Hubbard model
Physical Review B **97**, 165119 (2018).
Group(s): Werner / Project(s): DD5

Y. Murakami, M. Eckstein, and P. Werner
High-Harmonic Generation in Mott Insulators
Physical Review Letters **121**, 057405 (2018).
Group(s): Werner / Project(s): DD5

M. Schüler, Y. Murakami, and P. Werner
Nonthermal switching of charge order: Dynamical slowing down and optimal control
Physical Review B **97**, 155136 (2018).
Group(s): Werner / Project(s): DD5

A. Herrmann, Y. Murakami, M. Eckstein, and P. Werner
Floquet prethermalization in the resonantly driven Hubbard model
Europhysics Letters **120**, 57001 (2017).
Group(s): Werner / Project(s): DD5

M. Schüler and Y. Pavlyukh
Spectral properties from Matsubara Green's function approach: Application to molecules
Physical Review B **97**, 115164 (2018).
Group(s): Werner / Project(s): DD5

Group of Oleg Yazyev

C.-J. Yi, B. Q. Lv, Q. S. Wu, B.-B. Fu, X. Gao, M. Yang, X.-L. Peng, M. Li, Y.-B. Huang, P. Richard, M. Shi, G. Li, O. V. Yazyev, Y.-G. Shi, T. Qian, and H. Ding
Observation of a nodal chain with Dirac surface states in TiB_2
Physical Review B **97**, 201107(R) (2018).
Group(s): Shi, Yazyev / Project(s): DD6

N. Xu, Y. T. Qian, Q. S. Wu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, V. N. Strocov, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, O. V. Yazyev, T. Qian, H. Ding, J. Mesot, and M. Shi
Trivial topological phase of CaAgP and the topological nodal-line transition in $CaAg(P_{1-x}As_x)$
Physical Review B **97**, 161111(R) (2018).
Group(s): Shi, Yazyev / Project(s): PP7, DD6

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

S. Zhang, Q. Wu, Y. Liu, and O. V. Yazyev
Magnetoresistance from Fermi Surface Topology
Physical Review B **99**, 035142 (2019).
Group(s): Yazyev / Project(s): DD6

M. M. Ugeda, A. Pulkin, S. Tang, H. Ryu, Q. Wu, Y. Zhang, D. Wong, Z. Pedramrazi, A. Martín-Recio, Y. Chen, F. Wang, Z.-X. Shen, S.-K. Mo, O. V. Yazyev, and M. F. Crommie
Observation of topologically protected states at crystalline phase boundaries in single-layer WSe_2
Nature Communications **9**, 3401 (2018).
Group(s): Yazyev / Project(s): DD6

X. Zhou, Q. Liu, Q. Wu, T. Nummy, H. Li, J. Griffith, S. Parham, J. Waugh, E. Emmanouilidou, B. Shen, O. V. Yazyev, N. Ni, and D. Dessau
Coexistence of tunable Weyl points and topological nodal lines in ternary transition-metal telluride $TaIrTe_4$
Physical Review B **97**, 241102(R) (2018).
Group(s): Yazyev / Project(s): DD6

J. Du, Z. Lou, S. Zhang, Y. Zhou, B. Xu, Q. Chen, Y. Tang, S. Chen, H. Chen, Q. Zhu, H. Wang, J. Yang, Q. Wu, O. V. Yazyev, and M. Fang
Extremely large magnetoresistance in the topologically trivial semimetal α-WP_2
Physical Review B **97**, 245101 (2018).
Group(s): Yazyev / Project(s): DD6

S. Roth, H. Lee, A. Sterzi, M. Zacchigna, A. Politano, R. Sankar, F. C. Chou, G. Di Santo, L. Petaccia, O. V. Yazyev, and A. Crepaldi
Reinvestigating the surface and bulk electronic properties of Cd_3As_2
Physical Review B **97**, 165439 (2018).
Group(s): Yazyev / Project(s): DD6

A. Crepaldi, G. Autès, G. Gatti, S. Roth, A. Sterzi, G. Manzoni, M. Zacchigna, C. Cacho, R. T. Chapman, E. Springate, E. A. Seddon, P. Bugnon, A. Magrez, H. Berger, I. Vobornik, M. Kalläne, A. Quer, K. Rossnagel, F. Parmigiani, O. V. Yazyev, and M. Grioni
Enhanced ultrafast relaxation rate in the Weyl semimetal phase of $MoTe_2$ measured by time- and angle-resolved photoelectron spectroscopy
Physical Review B **96**, 241408(R) (2017).
Group(s): Yazyev / Project(s): DD6

W. Zhang, Q. Wu, O. V. Yazyev, H. Weng, Z. Guo, W.-D. Cheng, and G.-L. Chai
Topological phase transitions driven by strain in monolayer tellurium
Physical Review B **98**, 115411 (2018).
Group(s): Yazyev / Project(s): DD6

E. Martino, A. Arakcheeva, G. Autès, A. Pisoni, M. D. Bachmann, K. A. Modic, T. Helm, O. V. Yazyev, P. J. W. Moll, L. Forró, and S. Katrych
$Sr_2Pt_{8-x}As$: a layered incommensurately modulated metal with saturated resistivity
IUCrJ **5**, 470 (2018).
Group(s): Yazyev / Project(s): DD6

G. Autès and O. V. Yazyev
Discovery of novel topological materials via high-throughput computational search
in *Computational Materials Discovery*, A. R. Oganov, G. Saleh, and A. G. Kvashnin, eds. (Royal Society of Chemistry, 2019), p. 392.
Group(s): Yazyev / Project(s): DD6

X.-L. He, X. Dong, Q. Wu, Z. Zhao, Q. Zhu, A. R. Oganov, Y. Tian, D. Yu, X.-F. Zhou, and H.-T. Wang
Predicting the ground-state structure of sodium boride
Physical Review B **97**, 100102(R) (2018).
Group(s): Yazyev / Project(s): DD6

Phase I PIs, not active in phase II

Group of Raffaella Buonsanti

J. Huang, N. Hörmann, E. Oveisi, A. Loiudice, G. L. De Gregorio, O. Andreussi, N. Marzari, and R. Buonsanti
Potential-induced nanoclustering of metallic catalysts during electrochemical CO_2 reduction
Nature Communications **9**, 3117 (2018).
Group(s): Buonsanti, Marzari / Project(s): PP7, Inc1

J. Wiktor, I. Reshetnyak, M. Strach, M. Scarongella, R. Buonsanti, and A. Pasquarello
Sizable excitonic effects undermining the photocatalytic efficiency of β-$Cu_2V_2O_7$
The Journal of Physical Chemistry Letters **9**, 5698 (2018).
Group(s): Buonsanti, Pasquarello / Project(s): VP2, PP7, DD4

Group of Claudia Cancellieri

M. González-Castaño, M. Döbeli, V. Araullo-Peters, L. P. H. Jeurgens, P. Schmutz, and C. Cancellieri
Substrate Purity Effect on the Defect Formation and Properties of Amorphous Anodic Barrier Al_2O_3
Journal of The Electrochemical Society **165**, C422 (2018).
Group(s): Cancellieri / Project(s): PP7

Group of Antoine Georges

M. Schüler, O. E. Peil, G. J. Kraberger, R. Pordzik, M. Marsman, G. Kresse, T. O. Wehling, and M. Aichhorn
Charge self-consistent many-body corrections using optimized projected localized orbitals
Journal of Physics: Condensed Matter **30**, 475901 (2018).
Group(s): Georges / Project(s): VP1

S. Riccò, M. Kim, A. Tamai, S. M. Walker, F. Y. Bruno, I. Cucchi, E. Cappelli, C. Besnard, T. K. Kim, P. Dudin, M. Hoesch, M. J. Gutmann, A. Georges, R. S. Perry, and F. Baumberger
In situ strain tuning of the metal-insulator-transition of Ca_2RuO_4 in angle-resolved photoemission experiments
Nature Communications **9**, 4535 (2018).
Group(s): Georges / Project(s): VP1

A. Moutenet, A. Georges, and M. Ferrero
Pseudogap and electronic structure of electron-doped Sr_2IrO_4
Physical Review B **97**, 155109 (2018).
Group(s): Georges / Project(s): VP1

M. Kim, J. Mravlje, M. Ferrero, O. Parcollet, and A. Georges
Spin-Orbit Coupling and Electronic Correlations in Sr_2RuO_4
Physical Review Letters **120**, 126401 (2018).
Group(s): Georges / Project(s): VP1

D. Hügel, H. U. R. Strand, and L. Pollet
Self-energy functional theory with symmetry breaking for disordered lattice bosons
Quantum Science and Technology **3**, 034006 (2018).
Group(s): Georges / Project(s): VP1

M. Kim
Signatures of spin-orbital states of t_{2g}^2 system in optical conductivity: RVO_3 (R = Y and La)
Physical Review B **97**, 155141 (2018).
Group(s): Georges / Project(s): VP1

Group of Christoph Koch

A. Shaikhha, Y. Klonatos, and C. Koch

Building Efficient Query Engines in a High-Level Language

ACM Transactions on Database Systems **43**, 4 (2018).

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

Group of Thomas Lippert

D. Pergolesi, E. Gilardi, E. Fabbri, V. Roddatis, G. F. Harrington, T. Lippert, J. A. Kilner, and E. Traversa

Interface Effects on the Ionic Conductivity of Doped Ceria–Yttria-Stabilized Zirconia Heterostructures

ACS Applied Materials & Interfaces **10**, 14160 (2018).

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

F. Haydous, W. Si, V. A. Guzenko, F. Waag, E. Pomjakushina, M. El Kazzi, L. Sévery, A. Wokaun, D. Pergolesi, and T. Lippert

Improved Photoelectrochemical Water Splitting of $CaNbO_2N$ Photoanodes by CoPi Photodeposition and Surface Passivation

The Journal of Physical Chemistry C **123**, 1059 (2019).

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

Group of Wendy Queen

M. Asgari, S. Jawahery, E. D. Bloch, M. R. Hudson, R. Flacau, B. Vlaisavljevich, J. R. Long, C. M. Brown, and W. L. Queen

An experimental and computational study of CO_2 adsorption in the sodalite-type M-BTT (M = Cr, Mn, Fe, Cu) metal–organic frameworks featuring open metal sites

Chemical Science **9**, 4579 (2018).

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

D. T. Sun, L. Peng, W. S. Reeder, S. M. Moosavi, D. Tiana, D. K. Britt, E. Oveisi, and W. L. Queen

Rapid, Selective Heavy Metal Removal from Water by a Metal–Organic Framework/Polydopamine Composite

ACS Central Science **4**, 349 (2018).

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

S. Yang, L. Peng, E. Oveisi, S. Bulut, D. T. Sun, M. Asgari, O. Trukhina, and W. L. Queen

MOF-Derived Cobalt Phosphide/Carbon Nanocubes for Selective Hydrogenation of Nitroarenes to Anilines

Chemistry–A European Journal **24**, 4234 (2018).

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

Group of Ursula Röthlisberger

J. A. Flores-Livas, D. Tomerini, M. Amsler, A. Boziki, U. Rothlisberger, and S. Goedecker

Emergence of hidden phases of methylammonium lead iodide ($CH_3NH_3PbI_3$) upon compression

Physical Review Materials **2**, 085201 (2018).

Group(s): Goedecker, Röthlisberger / Project(s): DD1, VP2, HP4

E. Bozkurt, M. A. S. Perez, R. Hovius, N. J. Browning, and U. Rothlisberger

Genetic Algorithm Based Design and Experimental Characterization of a Highly Thermostable Metalloprotein

Journal of the American Chemical Society **140**, 4517 (2018).

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

Group of Marta Rossell

M. Campanini, R. Erni, C.-H. Yang, R. Ramesh, and M. D. Rossell

Periodic Giant Polarization Gradients in Doped $BiFeO_3$ Thin Films

Nano Letters **18**, 717 (2018).

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

Group of Thomas J. Schmidt

B.-J. Kim, X. Cheng, D. F. Abbott, E. Fabbri, F. Bozza, T. Graule, I. E. Castelli, L. Wiles, N. Danilovic, K. E. Ayers, N. Marzari, and T. J. Schmidt

Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+\delta}$ and $PrBaCo_2O_{5+\delta}$

Advanced Functional Materials **28**, 1804355 (2018).

Group(s): Marzari, Schmidt / Project(s): PP7, Inc1

X. Cheng, E. Fabbri, Y. Yamashita, I. E. Castelli, B. Kim, M. Uchida, R. Haumont, I. Puente-Orench, and T. J. Schmidt

Oxygen Evolution Reaction on Perovskites: A Multieffect Descriptor Study Combining Experimental and Theoretical Methods

ACS Catalysis **8**, 9567 (2018).

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

Group of Thorsten Schmitt

D. E. McNally, X. Lu, J. Pelliciari, S. Beck, M. Dantz, M. Naamneh, T. Shang, M. Medarde, C. W. Schneider, V. N. Strocov, E. V. Pomjakushina,

C. Ederer, M. Radovic, and T. Schmitt
Electronic localization in $CaVO_3$ films via bandwidth control
npj Quantum Materials **4**, 6 (2019).
Group(s): Ederer, Medarde, Schmitt / Project(s): PP7

D. Meyers, K. Nakatsukasa, S. Mu, L. Hao, J. Yang, Y. Cao, G. Fabbris, H. Miao, J. Pelliciari, D. McNally, M. Dantz, E. Paris, E. Karapetrova, Y. Choi, D. Haskel, P. Shafer, E. Arenholz, T. Schmitt, T. Berlijn, S. Johnston, J. Liu, and M. P. M. Dean
Decoupling Carrier Concentration and Electron-Phonon Coupling in Oxide Heterostructures Observed with Resonant Inelastic X-Ray Scattering
Physical Review Letters **121**, 236802 (2018).
Group(s): Schmitt / Project(s): PP7

L. Das, F. Forte, R. Fittipaldi, C. G. Fatuzzo, V. Granata, O. Ivashko, M. Horio, F. Schindler, M. Dantz, Y. Tseng, D. E. McNally, H. M. Rønnow, W. Wan, N. B. Christensen, J. Pelliciari, P. Olalde-Velasco, N. Kikugawa, T. Neupert, A. Vecchione, T. Schmitt, M. Cuoco, and J. Chang
Spin-Orbital Excitations in Ca_2RuO_4 Revealed by Resonant Inelastic X-Ray Scattering
Physical Review X **8**, 011048 (2018).
Group(s): Schmitt / Project(s): PP7

U. Maitra, R. A. House, J. W. Somerville, N. Tapia-Ruiz, J. G. Lozano, N. Guerrini, R. Hao, K. Luo, L. Jin, M. A. Pérez-Osorio, F. Massel, D. M. Pickup, S. Ramos, X. Lu, D. E. McNally, A. V. Chadwick, F. Giustino, T. Schmitt, L. C. Duda, M. R. Roberts, and P. G. Bruce
Oxygen redox chemistry without excess alkali-metal ions in $Na_{2/3}[Mg_{0.28}Mn_{0.72}]O_2$
Nature Chemistry **10**, 288 (2018).
Group(s): Schmitt / Project(s): PP7

S. Kang, Y. Tseng, B. H. Kim, S. Yun, B. Sohn, B. Kim, D. McNally, E. Paris, C. H. Kim, C. Kim, T. W. Noh, S. Ishihara, T. Schmitt, and J.-G. Park
Orbital-selective confinement effect of Ru 4d orbitals in $SrRuO_3$ ultrathin film
Physical Review B **99**, 045113 (2019).
Group(s): Schmitt / Project(s): PP7

M. Kang, J. Pelliciari, Y. Krockenberger, J. Li, D. E. McNally, E. Paris, R. Liang, W. N. Hardy, D. A. Bonn, H. Yamamoto, T. Schmitt, and R. Comin
Resolving the nature of electronic excitations in resonant inelastic x-ray scattering
Physical Review B **99**, 045105 (2019).
Group(s): Schmitt / Project(s): PP7

Group of Grigory Smolentsev

G. Smolentsev, M. A. Soldatov, B. Probst, C. Bachmann, N. Azzaroli, R. Alberto, M. Nachtegaal, and J. A. van Bokhoven
Structure of the Co^I Intermediate of a Cobalt Pentapyridyl Catalyst for Hydrogen Evolution Revealed by Time-Resolved X-ray Spectroscopy
ChemSusChem **11**, 3087 (2018).
Group(s): Smolentsev / Project(s): PP7

G. Smolentsev, K. M. van Vliet, N. Azzaroli, J. A. van Bokhoven, A. M. Brouwer, B. de Bruin, M. Nachtegaal, and M. Tromp
Pump-probe XAS investigation of the triplet state of an Ir photosensitizer with chromenopyridinone ligands
Photochemical & Photobiological Sciences **17**, 896 (2018).
Group(s): Smolentsev / Project(s): PP7

Group of Urs Staub

M. Porer, M. Fechner, E. M. Bothschafter, L. Rettig, M. Savoini, V. Esposito, J. Rittmann, M. Kubli, M. J. Neugebauer, E. Abreu, T. Kubacka, T. Huber, G. Lantz, S. Parchenko, S. Grübel, A. Paarmann, J. Noack, P. Beaud, G. Ingold, U. Aschauer, S. L. Johnson, and U. Staub
Ultrafast Relaxation Dynamics of the Antiferrodistortive Phase in Ca Doped $SrTiO_3$
Physical Review Letters **121**, 055701 (2018).
Group(s): Aschauer, Staub / Project(s): PP7, DD5

N. S. Fedorova, Y. W. Windsor, C. Findler, M. Ramakrishnan, A. Bortis, L. Rettig, K. Shimamoto, E. M. Bothschafter, M. Porer, V. Esposito, Y. Hu, A. Alberca, T. Lippert, C. W. Schneider, U. Staub, and N. A. Spaldin
Relationship between crystal structure and multiferroic orders in orthorhombic perovskite manganites
Physical Review Materials **2**, 104414 (2018).
Group(s): Spaldin, Staub / Project(s): PP7, VP1, DD5

C. Dornes, Y. Acremann, M. Savoini, M. Kubli, M. J. Neugebauer, E. Abreu, L. Huber, G. Lantz, C. A. F. Vaz, H. Lemke, E. M. Bothschafter, M. Porer,

V. Esposito, L. Rettig, M. Buzzi, A. Alberca, Y. W. Windsor, P. Beaud, U. Staub, D. Zhu, S. Song, J. M. Glownia, and S. L. Johnson

The ultrafast Einstein–de Haas effect

Nature **565**, 209 (2019).

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

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

Physical Review X **8**, 011005 (2018).

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

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

Neural-network quantum state tomography

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

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

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

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

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

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

Q. Wu, C. Piveteau, Z. Song, and O. V. Yazyev

$MgTa_2N_3$: A reference Dirac semimetal

Physical Review B **98**, 081115(R) (2018).

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

2. Scientific articles in journals without peer review

Group of Ulrich Aschauer

C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer
Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$
arXiv:1811.10858 (2018).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

Group of Clémence Corminboeuf

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

Group of Claude Ederer

A. Hampel, P. Liu, C. Franchini, and C. Ederer
Energetics of the coupled electronic-structural transition in the rare-earth nickelates
arXiv:1807.03524 (2018).
Group(s): Ederer / Project(s): DD5

O. E. Peil, A. Hampel, C. Ederer, and A. Georges
Mechanism and control parameters of the metal-insulator transition in nickelates
arXiv:1809.03720 (2018).
Group(s): Ederer, Georges / Project(s): VP1, DD5

Group of Stefan Goedecker

O. Andreussi, N. G. Hörmann, F. Nattino, G. Fisicaro, S. Goedecker, and N. Marzari
Solvent-aware Interfaces in Continuum Solvation
arXiv:1901.08138 (2019).
Group(s): Goedecker, Marzari / Project(s): DD1, DD3

Group of Jürg Hutter

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

Group of Teodoro Laino

M. Mottet, A. Marcolongo, T. Laino, and I. Tavernelli
Doping in garnet-type electrolytes: Kinetic and thermodynamic effects from molecular dynamics simulations
ChemRxiv. Preprint (2019), doi:10.26434/chemrxiv.7628771.v1.
Group(s): Laino, Tavernelli / Project(s): Inc1

T. Binninger, A. Marcolongo, V. Weber, and T. Laino
Potential window of stable stoichiometry of solid-state electrolyte materials
arXiv:1901.02251 (2019).
Group(s): Laino / Project(s): Inc1

Group of Nicola Marzari

G. Prandini, M. Galante, N. Marzari, and P. Umari
SIMPLE code: optical properties with optimal basis functions
arXiv:1901.03175 (2019).
Group(s): Marzari / Project(s): DD3

M. Simoncelli, N. Marzari, and F. Mauri
Unified theory of thermal transport in crystals and disordered solids
arXiv:1901.01964 (2019).
Group(s): Marzari / Project(s): DD3

C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, and U. Aschauer
Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$
arXiv:1811.10858 (2018).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

M. Cococcioni and N. Marzari
Energetics and cathode voltages of $LiMPO_4$ olivines (M = Fe, Mn) from extended Hubbard functionals
arXiv:1811.06586 (2018).
Group(s): Marzari / Project(s): Inc1

N. Colonna, N. L. Nguyen, A. Ferretti, and N. Marzari
Koopmans-compliant functionals and potentials and their application to the GW100 test-set
arXiv:1810.02111 (2018).
Group(s): Marzari / Project(s): HP3

A. Cepellotti and N. Marzari
On the Kinetic Theory of Thermal Transport in Crystals
in *Handbook of Materials Modeling: Applications:*

Current and Emerging Materials, W. ANDREONI AND S. YIP, eds. (Springer, Cham, 2018), pp. 1–42.

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

O. ANDREUSSI, N. G. HÖRMANN, F. NATTINO, G. FISICARO, S. GOEDECKER, AND N. MARZARI
Solvent-aware Interfaces in Continuum Solvation
arXiv:1901.08138 (2019).

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

Group of Michele Parrinello

S. PÉREZ-CONESA, P. M. PIAGGI, AND M. PARRINELLO
A local fingerprint for hydrophobicity and hydrophilicity: from methane to peptides
arXiv:1808.09712 (2018).

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

O. VALSSON AND M. PARRINELLO
Variationally Enhanced Sampling
in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. ANDREONI AND S. YIP, eds. (Springer, Cham, 2018), pp. 1–14.

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

Group of Daniele Passerone

L. TALIRZ AND C. A. PIGNEDOLI
Electronic Structure of Atomically Precise Graphene Nanoribbons
in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. ANDREONI AND S. YIP, eds. (Springer, Cham, 2018), pp. 1–35.

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

Group of Giovanni Pizzi

G. PIZZI, A. TOGO, AND B. KOZINSKY
Provenance, workflows, and crystallographic tools in materials science: AiiDA, spglib, and seekpath
MRS Bulletin **43**, 696 (2018).

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

G. PIZZI
Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud
in *Handbook of Materials Modeling : Methods: Theory and Modeling*, W. ANDREONI AND S. YIP, eds. (Springer, Cham, 2018), pp. 1–24.

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

Group of Oleg Yazyev

M. YAO, H. LEE, N. XU, Y. WANG, J. MA, O. V. YAZYEV, Y. XIONG, M. SHI, G. AEPPLI, AND Y. SOH
Switchable Weyl nodes in topological Kagome ferromagnet Fe_3Sn_2
arXiv:1810.01514 (2018).

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

Group of Berend Smit

L. TALIRZ AND C. A. PIGNEDOLI
Electronic Structure of Atomically Precise Graphene Nanoribbons
in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, W. ANDREONI AND S. YIP, eds. (Springer, Cham, 2018), pp. 1–35.

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

Group of Alexey Soluyanov

Q. WU, A. A. SOLUYANOV, AND T. BZDUŠEK
Beyond the Tenfold Way: Non-Abelian Topology in Noninteracting Metals
arXiv:1808.07469 (2018).

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

G. W. WINKLER, A. E. ANTIPOV, B. VAN HECK, A. A. SOLUYANOV, L. I. GLAZMAN, M. WIMMER, AND R. M. LUTCHYN
A unified numerical approach to semiconductor-superconductor heterostructures
arXiv:1810.04180 (2018).

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

Group of Ivano Tavernelli

M. MOTTET, A. MARCOLONGO, T. LAINO, AND I. TAVERNELLI
Doping in garnet-type electrolytes: Kinetic and thermodynamic effects from molecular dynamics simulations
ChemRxiv. Preprint (2019), doi:10.26434/chemrxiv.7628771.v1.

Group(s): Laino, Tavernelli / Project(s): Inc1

Group of Anatole von Lilienfeld

G. F. VON RUDORFF AND O. A. VON LILIENFELD
Alchemical perturbation density functional theory for rapid yet accurate quantum property estimates
arXiv:1809.01647 (2018).

Group(s): von Lilienfeld / Project(s): Inc2

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

Group of Oleg Yazyev

D. Gosálbez-Martínez, G. Autès, and O. V. Yazyev
Topological Fermi-arc surface resonances in bcc iron
arXiv:1811.08178 (2018).
Group(s): Yazyev / Project(s): DD6

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

R. Fournier, L. Wang, O. V. Yazyev, and Q. Wu
An Artificial Neural Network Approach to the Analytic Continuation Problem
arXiv:1810.00913 (2018).
Group(s): Yazyev / Project(s): DD6

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

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

Group of Antoine Georges

O. E. Peil, A. Hampel, C. Ederer, and A. Georges
Mechanism and control parameters of the metal-insulator transition in nickelates
arXiv:1809.03720 (2018).
Group(s): Ederer, Georges / Project(s): VP1, DD5

3. Publications involving several groups

M. Porer, M. Fechner, E. M. Bothschafter, L. Rettig, M. Savoini, V. Esposito, J. Rittmann, M. Kubli, M. J. Neugebauer, E. Abreu, T. Kubacka, T. Huber, G. Lantz, S. Parchenko, S. Grübel, A. Paarmann, J. Noack, P. Beaud, G. Ingold, U. Aschauer, S. L. Johnson, and U. Staub

Ultrafast Relaxation Dynamics of the Antiferrodistortive Phase in Ca Doped $SrTiO_3$

Physical Review Letters **121**, 055701 (2018).

Group(s): Aschauer, Staub / Project(s): PP7, DD5

J. Huang, N. Hörmann, E. Oveisi, A. Loiudice, G. L. De Gregorio, O. Andreussi, N. Marzari, and R. Buonsanti

Potential-induced nanoclustering of metallic catalysts during electrochemical CO_2 reduction

Nature Communications **9**, 3117 (2018).

Group(s): Buonsanti, Marzari / Project(s): PP7, Inc1

J. Wiktor, I. Reshetnyak, M. Strach, M. Scarongella, R. Buonsanti, and A. Pasquarello

Sizable excitonic effects undermining the photocatalytic efficiency of β-$Cu_2V_2O_7$

The Journal of Physical Chemistry Letters **9**, 5698 (2018).

Group(s): Buonsanti, Pasquarello / Project(s): VP2, PP7, DD4

V. Kapil, M. Rossi, O. Marsalek, R. Petraglia, Y. Litman, T. Spura, B. Cheng, A. Cuzzocrea, R. H. Meissner, D. M. Wilkins, B. A. Helfrecht, P. Juda, S. P. Bienvenue, W. Fang, J. Kessler, I. Poltavsky, S. Vandenbrande, J. Wieme, C. Corminboeuf, T. D. Kühne, D. E. Manolopoulos, T. E. Markland, J. O. Richardson, A. Tkatchenko, G. A. Tribello, V. V. Speybroeck, and M. Ceriotti

i-PI 2.0: A universal force engine for advanced molecular simulations

Computer Physics Communications (2018), doi:10.1016/j.cpc.2018.09.020.

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

L. Vannay, B. Meyer, R. Petraglia, G. Sforazzini, M. Ceriotti, and C. Corminboeuf

Analyzing Fluxional Molecules Using DORI

Journal of Chemical Theory and Computation **14**, 2370 (2018).

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

A. Grisafi, A. Fabrizio, B. Meyer, D. M. Wilkins, C. Corminboeuf, and M. Ceriotti

Transferable Machine-Learning Model of the Electron Density

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

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

M. Busch, A. Fabrizio, S. Luber, J. Hutter, and C. Corminboeuf

Exploring the Limitation of Molecular Water Oxidation Catalysts

The Journal of Physical Chemistry C **122**, 12404 (2018).

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

B. Meyer, B. Sawatlon, S. Heinen, O. A. von Lilienfeld, and C. Corminboeuf

Machine learning meets volcano plots: computational discovery of cross-coupling catalysts

Chemical Science **9**, 7069 (2018).

Group(s): Corminboeuf, von Lilienfeld / Project(s): DD1, Inc2

F. Maresca, D. Dragoni, G. Csányi, N. Marzari, and W. A. Curtin

Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential

npj Computational Materials **4**, 69 (2018).

Group(s): Curtin, Marzari / Project(s): DD2

D. E. McNally, X. Lu, J. Pelliciari, S. Beck, M. Dantz, M. Naamneh, T. Shang, M. Medarde, C. W. Schneider, V. N. Strocov, E. V. Pomjakushina, C. Ederer, M. Radovic, and T. Schmitt

Electronic localization in $CaVO_3$ films via bandwidth control

npj Quantum Materials **4**, 6 (2019).

Group(s): Ederer, Medarde, Schmitt / Project(s): PP7

O. Gröning, S. Wang, X. Yao, C. A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Müllen, P. Ruffieux, and R. Fasel

Engineering of robust topological quantum phases in graphene nanoribbons

Nature **560**, 209 (2018).

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

S. Mishra, M. Krzeszewski, C. A. Pignedoli, P. Ruffieux, R. Fasel, and D. T. Gryko

On-surface synthesis of a nitrogen-embedded buckybowl with inverse Stone-Thrower-Wales topology

Nature Communications **9**, 1714 (2018).

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

S. Mishra, T. G. Lohr, C. A. Pignedoli, J. Liu, R. Berger, J. I. Urgel, K. Müllen, X. Feng, P. Ruffieux, and R. Fasel
Tailoring Bond Topologies in Open-Shell Graphene Nanostructures
ACS Nano **12**, 11917 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

X.-Y. Wang, J. I. Urgel, G. B. Barin, K. Eimre, M. Di Giovannantonio, A. Milani, M. Tommasini, C. A. Pignedoli, P. Ruffieux, X. Feng, R. Fasel, K. Müllen, and A. Narita
Bottom-Up Synthesis of Heteroatom-Doped Chiral Graphene Nanoribbons
Journal of the American Chemical Society **140**, 9104 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

A. V. Yakutovich, J. Hoja, D. Passerone, A. Tkatchenko, and C. A. Pignedoli
Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111)
Journal of the American Chemical Society **140**, 1401 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

M. Di Giovannantonio, J. I. Urgel, U. Beser, A. V. Yakutovich, J. Wilhelm, C. A. Pignedoli, P. Ruffieux, A. Narita, K. Müllen, and R. Fasel
On-Surface Synthesis of Indenofluorene Polymers by Oxidative Five-Membered Ring Formation
Journal of the American Chemical Society **140**, 3532 (2018).
Group(s): Fasel, Passerone / Project(s): DD3

O. Andreussi and G. Fisicaro
Continuum embeddings in condensed-matter simulations
International Journal of Quantum Chemistry **119**, e25725 (2018).
Group(s): Goedecker, Marzari / Project(s): Inc1

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

D. Pergolesi, E. Gilardi, E. Fabbri, V. Roddatis, G. F. Harrington, T. Lippert, J. A. Kilner, and E. Traversa
Interface Effects on the Ionic Conductivity of Doped Ceria–Yttria-Stabilized Zirconia Heterostructures
ACS Applied Materials & Interfaces **10**, 14160 (2018).
Group(s): Lippert, Pergolesi / Project(s): PP7

F. Haydous, W. Si, V. A. Guzenko, F. Waag, E. Pomjakushina, M. El Kazzi, L. Sévery, A. Wokaun, D. Pergolesi, and T. Lippert
Improved Photoelectrochemical Water Splitting of $CaNbO_2N$ Photoanodes by CoPi Photodeposition and Surface Passivation
The Journal of Physical Chemistry C **123**, 1059 (2019).
Group(s): Lippert, Pergolesi / Project(s): PP7

Á. Szabó, C. Klinkert, D. Campi, C. Stieger, N. Marzari, and M. Luisier
Ab Initio Simulation of Band-to-Band Tunneling FETs With Single- and Few-Layer 2-D Materials as Channels
IEEE Transactions on Electron Devices **65**, 4180 (2018).
Group(s): Luisier, Marzari / Project(s): DD3

C. Klinkert, A. Szabo, D. Campi, C. Stieger, N. Marzari, and M. Luisier
Novel 2-D Materials for Tunneling FETs: an Ab-initio Study
in *2018 76th Device Research Conference (DRC)* (IEEE, 2018), pp. 1–2.
Group(s): Luisier, Marzari / Project(s): DD3

B.-J. Kim, X. Cheng, D. F. Abbott, E. Fabbri, F. Bozza, T. Graule, I. E. Castelli, L. Wiles, N. Danilovic, K. E. Ayers, N. Marzari, and T. J. Schmidt
Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+\delta}$ and $PrBaCo_2O_{5+\delta}$
Advanced Functional Materials **28**, 1804355 (2018).
Group(s): Marzari, Schmidt / Project(s): PP7, Inc1

C.-J. Yi, B. Q. Lv, Q. S. Wu, B.-B. Fu, X. Gao, M. Yang, X.-L. Peng, M. Li, Y.-B. Huang, P. Richard, M. Shi, G. Li, O. V. Yazyev, Y.-G. Shi, T. Qian, and H. Ding
Observation of a nodal chain with Dirac surface states in TiB_2
Physical Review B **97**, 201107(R) (2018).
Group(s): Shi, Yazyev / Project(s): DD6

N. Xu, Y. T. Qian, Q. S. Wu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, V. N. Strocov, E. Pomjakushina, K. Conder, N. C.

PLUMB, M. RADOVIC, O. V. YAZYEV, T. QIAN, H. DING, J. MESOT, AND M. SHI
Trivial topological phase of CaAgP and the topological nodal-line transition in CaAg($P_{1-x}As_x$)
Physical Review B **97**, 161111(R) (2018).
Group(s): Shi, Yazyev / Project(s): PP7, DD6

R. MERCADO, R.-S. FU, A. V. YAKUTOVICH, L. TALIRZ, M. HARANCZYK, AND B. SMIT
In Silico Design of 2D and 3D Covalent Organic Frameworks for Methane Storage Applications
Chemistry of Materials **30**, 5069 (2018).
Group(s): Smit, Pizzi / Project(s): DD4, OSP

S. KAMPOURI, T. N. NGUYEN, C. P. IRELAND, B. VALIZADEH, F. M. EBRAHIM, G. CAPANO, D. ONGARI, A. MACE, N. GUIJARRO, K. SIVULA, A. SIENKIEWICZ, L. FORRÓ, B. SMIT, AND K. C. STYLIANOU
Photocatalytic hydrogen generation from a visible-light responsive metal-organic framework system: the impact of nickel phosphide nanoparticles
Journal of Materials Chemistry A **6**, 2476 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

T. N. NGUYEN, S. KAMPOURI, B. VALIZADEH, W. LUO, D. ONGARI, O. M. PLANES, A. ZÜTTEL, B. SMIT, AND K. C. STYLIANOU
Photocatalytic Hydrogen Generation from a Visible-Light-Responsive Metal–Organic Framework System: Stability versus Activity of Molybdenum Sulfide Cocatalysts
ACS Applied Materials & Interfaces **10**, 30035 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

S. KAMPOURI, T. N. NGUYEN, M. SPODARYK, R. G. PALGRAVE, A. ZÜTTEL, B. SMIT, AND K. C. STYLIANOU
Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH_2 under Visible Light Irradiation
Advanced Functional Materials **28**, 1806368 (2018).
Group(s): Smit, Stylianou / Project(s): DD4

S. M. MOOSAVI, A. CHIDAMBARAM, L. TALIRZ, M. HARANCZYK, K. C. STYLIANOU, AND B. SMIT
Capturing chemical intuition in synthesis of metal-organic frameworks
Nature Communications **10**, 539 (2019).
Group(s): Smit, Stylianou / Project(s): DD4

N. S. FEDOROVA, Y. W. WINDSOR, C. FINDLER, M. RAMAKRISHNAN, A. BORTIS, L. RETTIG, K. SHIMAMOTO, E. M. BOTHSCHAFTER, M. PORER, V. ESPOSITO, Y. HU, A. ALBERCA, T. LIPPERT, C. W. SCHNEIDER, U. STAUB, AND N. A. SPALDIN
Relationship between crystal structure and multiferroic orders in orthorhombic perovskite manganites
Physical Review Materials **2**, 104414 (2018).
Group(s): Spaldin, Staub / Project(s): PP7, VP1, DD5

A. SCARAMUCCI, H. SHINAOKA, M. V. MOSTOVOY, M. MÜLLER, C. MUDRY, M. TROYER, AND N. A. SPALDIN
Multiferroic Magnetic Spirals Induced by Random Magnetic Exchanges
Physical Review X **8**, 011005 (2018).
Group(s): Spaldin, Troyer / Project(s): VP1

Q. WU, C. PIVETEAU, Z. SONG, AND O. V. YAZYEV
$MgTa_2N_3$: A reference Dirac semimetal
Physical Review B **98**, 081115(R) (2018).
Group(s): Troyer, Yazyev / Project(s): DD6

O. E. PEIL, A. HAMPEL, C. EDERER, AND A. GEORGES
Mechanism and control parameters of the metal-insulator transition in nickelates
arXiv:1809.03720 (2018).
Group(s): Ederer, Georges / Project(s): VP1, DD5

C. RICCA, I. TIMROV, M. COCOCCIONI, N. MARZARI, AND U. ASCHAUER
Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$
arXiv:1811.10858 (2018).
Group(s): Aschauer, Marzari / Project(s): DD5, DD3

O. ANDREUSSI, N. G. HÖRMANN, F. NATTINO, G. FISICARO, S. GOEDECKER, AND N. MARZARI
Solvent-aware Interfaces in Continuum Solvation
arXiv:1901.08138 (2019).
Group(s): Goedecker, Marzari / Project(s): DD1, DD3

M. YAO, H. LEE, N. XU, Y. WANG, J. MA, O. V. YAZYEV, Y. XIONG, M. SHI, G. AEPPLI, AND Y. SOH
Switchable Weyl nodes in topological Kagome ferromagnet Fe_3Sn_2
arXiv:1810.01514 (2018).
Group(s): Shi, Yazyev / Project(s): DD6

Cover picture

Symmetry-adapted machine learning predicts the electron charge density as a sum of atomic contributions, making it possible to train the model on smaller molecules and apply it to larger, flexible compounds (from Clémence Corminboeuf and Michele Ceriotti, EPFL, Design & Discovery Project 1 [7]).

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.