D9.4

MAX Impact Assessment Report, Final version

Silvana Muscella, Francesco Osimanti, Rita Giuffrida,
Maria Bartolacelli, Luisa Neri

Due date of deliverable:	30/09/2022	(**Month 46**)
Actual submission date:	18/10/2022	
Final version:	07/10/2022	

Lead beneficiary:	Trust-IT (participant number 14)
Dissemination level:	PU - Public

Document information

Project acronym:	MAX
Project full title:	Materials Design at the Exascale
Research Action Project type:	European Centre of Excellence in materials modelling, simulations and design
EC Grant agreement no.:	824143
Project starting / end date:	01/12/2018 (month 1) / 30/09/2022 (month 46)
Website:	www.max-centre.eu
Deliverable No.:	D9.4

Authors: S. Muscella, R. Giuffrida, F. Osimanti, (TRUST-IT); M. Bartolacelli, L. Neri (CNR)

To be cited as: S. Muscella et al., (2022): MAX Impact Assessment Report, Final version. Deliverable D9.4 of the H2020 project MAX (final version as of 07/10/2022). EC grant agreement no: 824143, Trust-IT, Pisa, Italy.

Table of Content

Versioning and contribution history

Version	Date	Author	Notes
0.1	01.07.2022	Francesco Osimanti, Rita Giuffrida (Trust-IT)	Table of Contents (ToC)
0.2	18.07.2022	Rita Giuffrida (Trust-IT)	Inputs in sections 1, and 2
0.3	19.07.2022	Rita Giuffrida (Trust-IT)	Inputs in sections 3 and 4
0.4	26.07.2022	Rita Giuffrida (Trust-IT)	Inputs in sections 5 and 6
0.5	08.08.2022	Francesco Osimanti (Trust-IT)	Revision of Sections 1, 2, 3, 4 and 5
0.6	10.08.2022	Rita Giuffrida (Trust-IT)	Inputs in Annex 1, 2 and 3
0.7	15.08.2022	Rita Giuffrida (Trust-IT)	Executive Summary and Conclusion
0.8	18.08.2022	Francesco Osimanti (Trust-IT)	Revision of the entire document and additional inputs in all the document sections
0.9	19.09.2022	Luisa Neri (CNR)	Revision of the document
1.0	04.10.2022	Luisa Neri, Maria Bartolacelli (CNR), Francesco Osimanti, Rita Giuffrida (Trust-IT)	Final adjustments to the document

List of figures.

List of tables.

Executive Summary

The deliverable D9.4 *Impact Assessment Report, Final Version* is the last dissemination and communication report developed by MAX and aims to present the main achievements and impact generated in terms of dissemination, communication and stakeholders engagement during the entire lifetime of the project. The report takes the legacy from the D9.2 "Impact Assessment Report, mid-term version" and D9.3 "MAX Communication and Dissemination Strategy and Stakeholder Engagement Plan, Final version" and presents the results of the strategies proposed in the previous two deliverables.

The deliverable presents the main activities and plans necessary to build a strong MAX community. For this purpose, the report presents the MAX stakeholder groups and targeted engagement activities. Moreover, the report presents practical key assets necessary to ensure visibility of MAX as a research and innovation action aimed at underpinning the project's sustainability path through its set of main outputs (flagship codes, workflows, services).

In terms of impact and reporting, the deliverable shows the main achievements gained in terms of website evolution and visits, scientific publications, participation in conferences and events, collaboration with relevant initiatives in the HPC ecosystem, and the size of the community reached. A set of KPIs are presented to show the impact generated by each of these activities.

This deliverable, initially planned to be released in M36, was postponed to M46, following the 10-month extension of the project. The project's activities were hit by COVID-19 and the extension allowed the team to postpone the organisation and joining of events, such as the MAX training schools and the participation to the Psi-K conference, which turned out to be useful engagement activities for the project's community.

1. Introduction

This report tracks the impact assessment coming from dissemination and communication activities and stakeholders' engagement performed by the MAX team, from M19 (June 2020) until September 2022 (M46).

The purpose of this report is to update the impact assessment report outlined in D9.2 (*Impact Assessment Report, mid-term version*) submitted in M18 and to show how MAX has positioned itself in the European HPC Centre of Excellence landscape. Hence, this report shows the tangible actions carried out by the project to maximise the adoption of its open-science exascale codes, to establish meaningful synergies with the HPC materials science community, to lower the gap in terms of skills development by engaging with academic, industrial players, European institutions and the general public.

The document is staggered into four main sections, defined as follows:

- **Section 2** provides an update of the illustrated strategy to efficiently monitor the impact of communication and dissemination activities;
- **Section 3** focuses on the sustainability path adopted by the project and the resulting impact on codes, workflows and services;
- **Section 4** presents the main stakeholder groups and the correlated strategies that have been leveraged to spark meaningful engagement;
- **Section 5** shows the impacts generated by communication and dissemination activities, across the spectrum of projects' channels and KPIs monitoring;
- **Section 6** draws the conclusions and summarises the main achievements throughout the entire project lifecycle;
- **Annex 1**: gives the list of acronyms;
- **Annex 2**: presents the list of scientific papers published by the MAX team;
- **Annex 3**: showcases the list of 3rd-party events joined by the MAX team.

2. Strategy for Impact Assessments of Communication and Dissemination activities

As outlined in D9.2, the MAX team has implemented communication, dissemination, and stakeholders engagement strategies, in order to successfully engage with the Stakeholder Groups described in Section 4. The key strategies, already presented in D9.2 and D9.3, are recapped as follows:

Strategy for Stakeholder Engagement

- Timely profiling of the community in conjunction with the addressed stakeholder group, tracking of the community development and growth over time, inclusive of attendees of third-party events and MAX webinars (see D9.1 and D9.3 to obtain more exhaustive details).
- Identification of the most suitable venues to drive stakeholder engagement, such as 3rd-party events, as well as hosting MAX webinar series and workshops.
- Event promotion and constant networking efforts through a wide array of digital channels and synergies with like-minded organisations, research and innovation projects and associations.
- Reporting on event outcomes, takeaways and impacts. This includes the development of ad-hoc reports that collect information about stakeholder categories, their geographical distribution, and

outcomes from Q&A and polls.

- Weekly social media activity and monitoring through the main social media platforms (LinkedIn and Twitter), both leveraged to boost the visibility and dissemination of the project outputs as well as to drive attention to events and training opportunities.
- Measuring overall impacts of engagement, including training.
- Strengthen collaborations with the HPC ecosystem in Europe.
- Engagement with women in technology and science.

Strategy for dissemination and communication

- Continuation of the communication strategy as outlined in *D9.3 MAX Communication and Dissemination Strategy and Stakeholder Engagement Plan*, which defines a set of KPIs against which corresponding impacts are monitored.
- Flexibility of the plan to be adapted as necessary to reflect project developments and in the face of ever-changing situations (such as the COVID-19 pandemic with event cancellations and postponements that affected the original envisaged plan as of M15).
- Increase in other forms of engagement, such as webinars, videos, Youtube training and events' playlists, newsletters to guarantee the chance for the community to keep up with new developments and opportunities, working closely with the synergies established.
- Carrying out large-scale promotional campaigns for the webinars across the MAX stakeholders' network and most influential synergies in the HPC ecosystem.
- Periodical update of the MAX website and impact measurement automatically generated through a purpose-built dashboard.
- Weekly campaigns on Twitter and LinkedIn, including SMART-based campaigns for events, with a clear start and end date and measurable targets to recruit prospective attendees, disseminate key-takeaways and provide live coverage of such events.
- Publication of scientific papers to highlight the MAX achievements in the scientific world.
- Measuring overall impacts of the communications strategy.

2.1 Engagement levers

The MAX Communication Methodology and Stakeholder Engagement Journey, visible in Figure 1, ensures that every single communication, dissemination and engagement activity is closely connected to the goals of the project.

The applied approach stems from the inbound methodology, which combines targeted content marketing, automation, SEO and other techniques, to strengthen the results of communication and engagement activities.

Every communication and dissemination activity is based on the concept of the ***"Attract – Convert – Close – Delight – Promote"*** process. This ensures a logical and seamless transition from **Stranger**, i.e., someone who is not familiar with the project, to **Visitor**, i.e., someone who start interacting and growing interest in the proposed content, to **Lead**, i.e. MAX target stakeholder who has shown interest in what the project communicates and disseminates and expressly requested MAX to engage with them. Then the Lead would turn into **Adopter**, i.e. a stakeholder who has actively participated in the project initiatives and interested in using its main results, and finally to **Promoter**, i.e., stakeholders who are so pleased with their interactions with MAX that they are happy to become actual ambassadors of the project's outputs, services and results. Promoters, in turn, are a key element to attract new strangers, who can start the cycle over.

While the phases from Attract to Convert are more focused on awareness raising and pure communication, the Close to Promote phases are fundamentally the expression of engagement actions.

The described process ensures an interconnected and efficient communications and engagement ecosystem.

Measuring feedback meaningfully through KPIs is an important step of the process as feedback can be used to take corrective actions needed to fruitfully activate the virtuous cycle (above described). Measurement can be achieved by organising important phases of the project as campaigns. Under each campaign, specific communication actions are planned and metrics are measured, which contribute to the achievement of the project's overall goals.

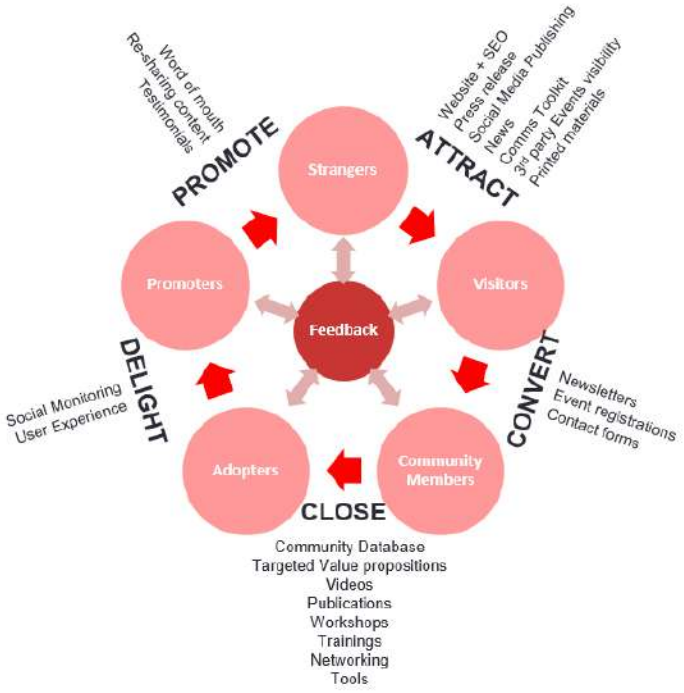


Figure 1. MAX communication and dissemination methodology and stakeholder journey.

3. MAX sustainability path and impact on codes, workflows and services

In order to evaluate the MAX impact, it is important to give an overview of the impact of exascale codes, workflows and services and assess sustainability path as some of the main outputs of the project. In particular, their evaluation include:

- European leadership in exascale and extreme-scale-oriented codes and innovative algorithms and/or solutions that address societal challenges or are important for key scientific and industrial applications in the materials domain;
- Improved access to computing applications and expertise that enables researchers and industry to be more productive, leading to scientific excellence and economic and social benefit;
- Improved competitiveness for European companies and SMEs through access to CoE expertise and services;
- Federating capabilities and integrating communities around computational science in Europe;

- A large number of scientists and engineers, in particular female and young ones, trained in the use of computational methods and optimisation of applications. As set out in the project, several measures have been planned in order to disseminate and exploit the results of MAX and to engage as much as possible the relevant communities. This is done by:
  - broadcasting of MAX results as broadly as possible across the European HPC ecosystem and beyond;
  - adopting a concerted approach to HPC skills development through an extensive training programme;
  - adopting a coordinated and collaborative approach in the EuroHPC context.

An overview of our sphere of influence is given below, and a more detailed description of our connection with the ecosystem is given in D10.6.

3.1 Flagships codes impact

The development of MAX flagship codes (Quantum ESPRESSO, SIESTA, CP2K, YAMBO, BigDft, FLEUR) in order to make them run on exascale hardware with high performance and throughput is the main output of the project. As an outcome of this porting we consider the impact on the different stakeholder groups, as identified in this report.

Impact of MAX flagships codes

As reported in the D9.2, the MAX flagship codes are able to run on hardware of the same type of the pre-exascale clusters. Codes have been strongly refactored and modularised and, at the same time, they continue to evolve rapidly with new capabilities. Importantly, all MAX codes are efficiently used in high-throughput workflows, thanks to the information and data platform AiiDA and Materials Cloud. In order to make them ready for exascale, in the last period we focused on the improvement of the GPU porting and finding solutions for easy portability. Now all the MAX codes are efficiently accelerated in the main core of the code and the complete porting will be available soon for the parts not yet publicly distributed. In addition, many solutions have been found and developed in order to guarantee an easy portability for the expected exascale evolution of architectures, for example through the use, and in some cases the development, of new libraries to facilitate the offloading.

This huge effort has allowed to strengthen the use and impact of MAX codes in the European and global landscape. As indicators of the impact of MAX flagship codes, we report:

- the number of code downloads, estimated to **> 10000 single downloads/year**
- the number of citations in scientific publications:
  - > **10500** publications in the period 2020 - September 2022, according to ISI citation index (6801 for Quantum ESPRESSO, 2397 for SIESTA, 1004 for CP2K, 280 for Yambo, 74 for BigDFT).
  - **179** additional citations refer to the AiiDA platform.

The first map below reports the *impact in different geographical regions*, sorting the number of papers citing the MAX flagship codes according to the European country in the affiliation (a country is counted once per paper even if in the affiliation of diverse authors).

The second map shows similar results at a global level.

Figure 2. Geographic distribution in Europe of author affiliations in papers citing the flagship codes (2020 - September 2022).

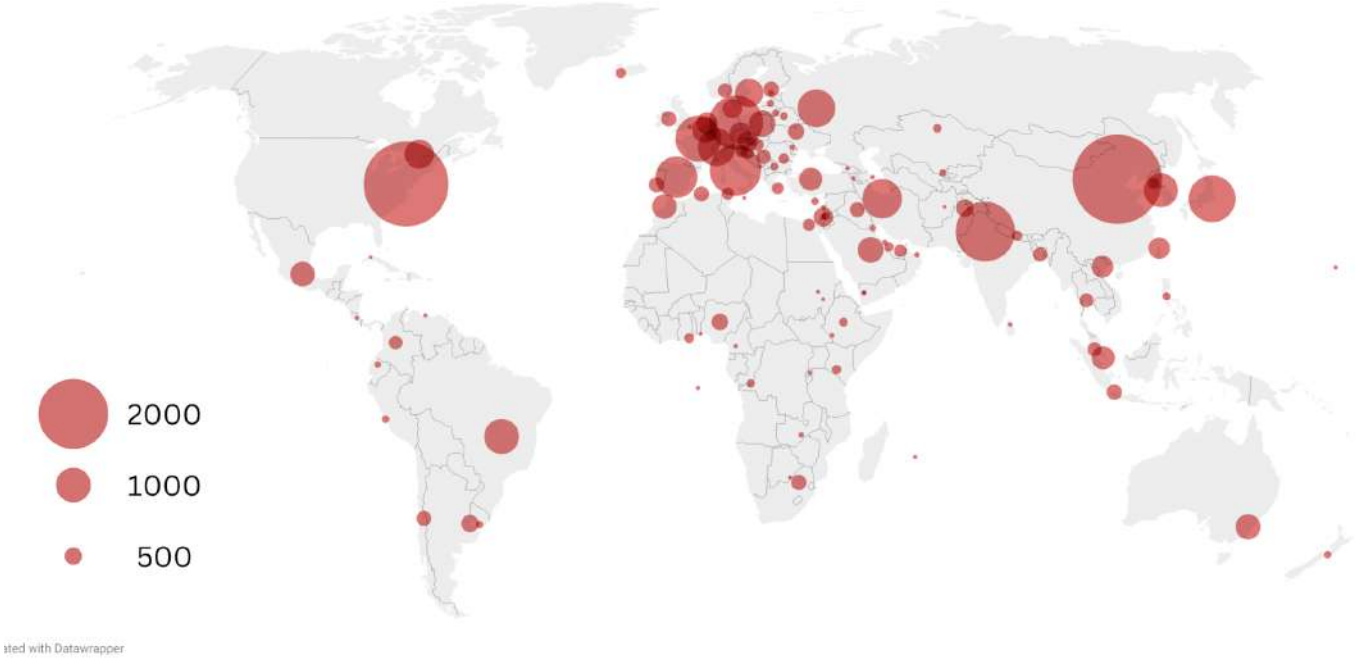


Figure 3. Geographic distribution all over the world of author affiliations in papers citing the flagship codes (2020 - September 2022).

- the number of community developers: **>100 active** involved across all the MAX flagship codes;
- The number and variety of training activities, which involved directly almost **1500 participants** (a detailed report about the activities and their evaluation is given in deliverable *D8.3 Second report on Training and Education*, M46), some of which we report here:
  - organization of 11 schools with hands-on sessions dedicated to the flagship codes, involving 1467

students; 3 more events are planned for the last 3 months of 2022 (see D8.3)
- organization of 5 Hackathons and workshops aimed at training code developers + 1 planned in October 2022;
- participation in schools organized by other institutions;
- contributions to 9 Master programmes with introductory courses on computational materials science, hands-on sessions on usage of MAX flagship codes and best practice in their usage in HPC facilities;
- 20 researchers hosted at MAX laboratories for basic and specialized training on MAX codes and libraries.

From a communication and dissemination point of view, several actions have been undertaken in order to push the benefits of MAX codes' adoption and usage.

1. A **webinar series on flagship codes** has been organized (see more details in section *5.6.2 MAX webinars* below): a webinar for each code has been organized, featuring a presentation of the code by its main developers, the latest achievements, and a Q&A session for users. The seven webinars ran from May to November 2020, and were attended globally by **900+ participants** from **66 countries**.

2. A dedicated event, **The MAX Happy Hour**, at the Psi-K conference (Lausanne, 23/8/2022) where the MAX partners and code developers met the users in the framework of the most important conference of the field. The event was attended by **200 participants**, 6% of which from industry. More details at Section 6 below.

3. A **"Software" area in the website**[1] has been set-up with rich information for the users. From the software page, sections on Codes, Libraries, Features and algorithms, Workflows are accessible, and always offer updated details on the codes. The section has received **1800+ visits** since the launch of the website.

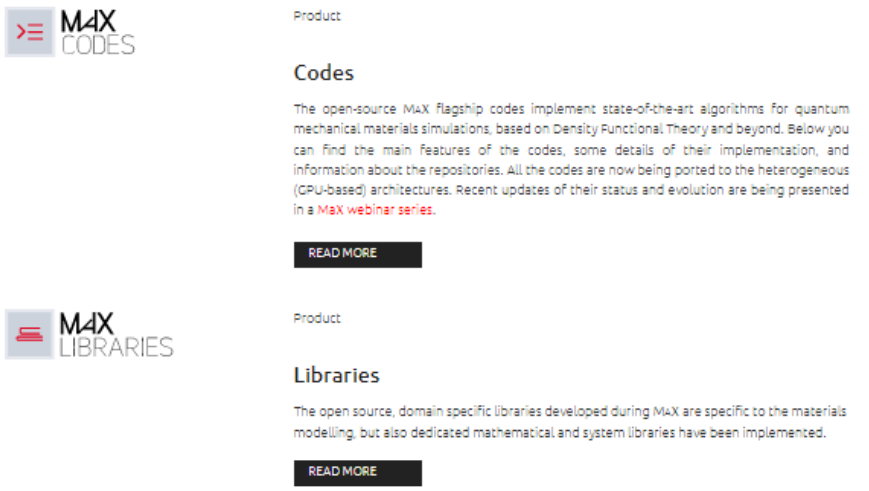


Figure 4. A section of The MAX website "Software" page, the gateway to several information on the codes and their impact.

[1] http://www.max-centre.eu/software

4. The **"Science & MAX section" of the website**[2], in which several publications from the CoE, and from outside, are presented, and sorted per code, in order to offer the users an access point to cutting-edge scientific and software developments. The section has received **1450+ visits**.

3.2 Automated workflow and data platform

MAX enables the evolution towards exascale computation also by supporting high-throughput automated workflows through AiiDA, which show a steady increase in adoption by its users. A comparison in figures between M19 and M46 is given. The numbers of packages and executable codes have risen from 45 and 80 in M19 to 83 and 120 in M46.

The list of plugin packages in the AiiDA registry[3] shows an average increase of 45%, as detailed below:

	plugins (M19, 05/2020)	packages (M19, 05/2020)	plugins (M46, 09/2022)	packages (M46, 09/2022)	plugins % growth	packages % growth
Calculations	89	35	127	53	42.70%	51.43%
Parsers	79	35	108	54	36.71%	54.29%
Data	61	21	92	27	50.82%	28.57%
Workflows	80	17	125	36	56.25%	111.76%
Others	114	22	99	29	-13.16%	31.82%

Table 1. The AiiDa registry values for M19 and M46, with growth percentages.

In addition, MAX, in collaboration with MARVEL, conceived and supports Materials Cloud[4], an Open Science Platform designed to enable seamless sharing of resources in computational materials science. Materials Cloud is connected to AiiDA, as calculations and workflows are openly available in its Explore section. The Materials Cloud statistics show the impact of this platform in the field of materials codes[5].

3.3 MAX Services

The MAX service activities are offered to a broad range of users, both academic and industrial. These services have been continuously improved during the duration of the project, to always guarantee users maximum support for exploiting at the best MAX codes on different kinds of architectures.

The main services offered are: i) the code and domain specific support for MAX codes; ii) the high level support, addressing more complex problem such for example the development of new features in MAX codes; iii) the support for the whole suite of AiiDA tools (i.e., AiiDAlab, quantum mobile, materials cloud); iv) the production of container-based deployment strategies to allow for easy access to codes and workflows of the MAX ecosystem.

[2] http://www.max-centre.eu/science-and-max/highlights
[3] https://aiidateam.github.io/aiida-registry/
[4] https://www.materialscloud.org/
[5] https://www.materialscloud.org/home#statistics

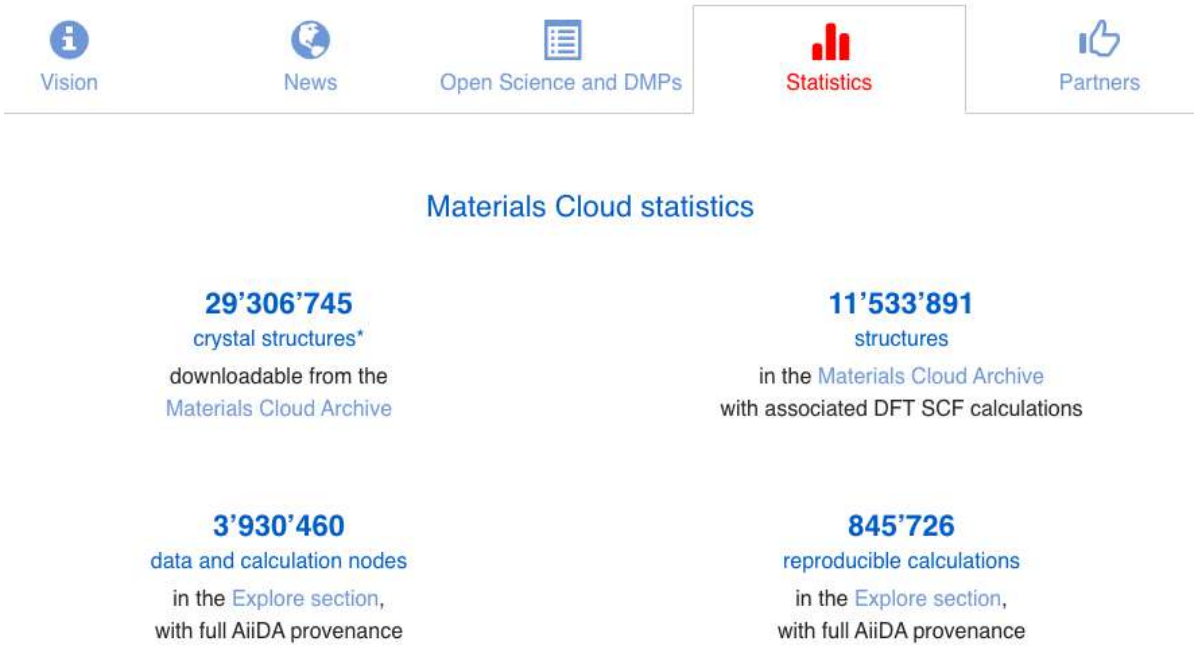


Figure 5. Materials Cloud statistics (September 2022).

The domain specific support is offered in two different ways: on one side, the support is offered by each code community through forum/mailing lists and some other channel (i.e., github threads, slack), where the responsible is always a specialist acting on behalf of MAX; on the other side, the support is explicitly operated through the MAX Help-desk. The latter offers both advanced support as well as a consultation for the utilisation of codes. Support to industries is also provided within this framework. As regarding the high level support requests they can be sent directly to the code communities support of each MAX code, via forums/mailing lists, filling a dedicated form on the web site or to the MAX Help-desk. Moreover both the Help-desk and each code community also offers support for using the containerised versions of MAX codes.

An updated and detailed report of MAX performed activities is given in *D7.3 Third (final) report on the activity of the High-Level Support services (third year)* (M46), we here point out some numbers to show the MAX impact and contribution to the users community.

- Support via forum or mailing list (M24-M46) by each MAX code community (in 46 months 7000+ queries solved):
  - 1500 threads, corresponding to a total of about 3000 emails/post,
  - 1300+ gitlab threads
  - 64 face-to-face support activities
  - 84000 slack messages
- Support operated by the MAX Help desk, including MAX and non-MAX codes (in 46 months, 840 support actions and 2794 emails, 51% for MAX codes and 49% for non MAX codes):

- 377 service support actions
- 1092 related emails

- high-level support (total in 46 months of 119 requests):
  - 60 support requests regarding, e.g., code usage on different architectures and requests for developing new features in MAX code, porting and benchmarking of MAX codes (esp. on GPUs).

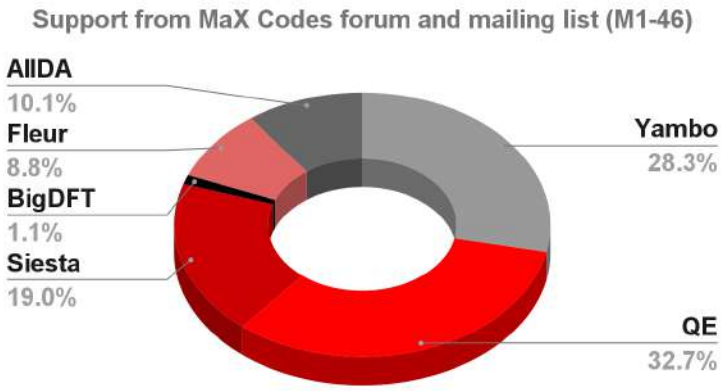


Figure 6. From D7.3: Percentage of email/forum threads for each MAX code M1-46.

4. Stakeholders groups and impact

Since the beginning of the project we pointed out several groups of stakeholders that could benefit from MAX activities, knowledge, and developments at different levels. Altogether they represent the ecosystem that may profit directly or indirectly from MAX results and outcomes, from the policy makers to the general public. Four main stakeholder groups (SGs) have thus been identified:

1. ***European institutions and ecosystems***: European institutions including policy makers and HPC projects and initiatives;
2. ***Industry***: specially independent software vendors, industrial end users of materials modelling, hardware manufacturers and integrators;
3. ***Research and academia institutions***: scientists and researchers interested in materials modelling, education system operating in the HPC and materials modelling ecosystems;
4. ***General public***: people with no technical background interested in learning about HPC, or scientific, project outcomes.

The MAX community amounts to around 4700 members in total, considering the sum of social media followers, newsletter subscribers, and MAX-organised events participants.

The figure below shows the current distribution of the Stakeholders Groups reached by the MAX team (HPC ecosystem, industrial and academic end-users, independent software vendors, code developers, large scale experimental facilities, EU and member states institutions, education system, and hardware manufacturers). The image does not include the general public, because while MAX has engaged with them, as explained in the paragraph 4.4, it was not possible to gather information about their size.

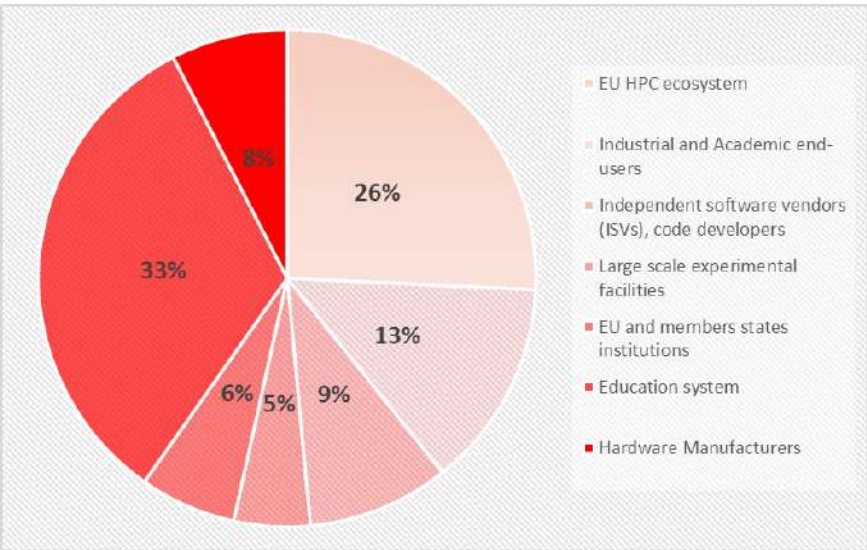


Figure 7. MAX Stakeholder's Community distribution.

The following sections present a short description of each SG and the targeted communication and dissemination strategy used to engage with them to ensure adequate awareness and knowledge of the main outcomes and uptake opportunities of the project.

4.1 European institutions and ecosystems

This SG is composed of European institutions and organizations/agencies that encompass policy makers and HPC projects and initiatives as well. The aim of engaging with them is related to sharing knowledge and trying to provide contextualized and strategic support for the development of future policies supposed to influence and affect the HPC environment. An extensive description of MAX activities in this field is given in *D10.6 Final report on MAX in the European, national, international HPC ecosystems* (M46).

The table below summarizes the main benefits and strategy adopted to engage with such SGs and offers an overview of the main undertaken actions.

Description and Driver of the SG	**Community and Networks**
Short description of the SG	Key European institutions involved in the HPC ecosystem with a view to capitalise on established networks and carry out joint dissemination towards scientific, research, industrial stakeholders and HPC-related projects and initiatives. Policy-driven synergy attained through the participation of MAX members with active roles within several boards and committees of such entities.

Benefits of cooperating with MAX	European institutions and ecosystems are interested in having a major stake in advanced computing capabilities and joint contributions to the HPC strategy.
Sample of community	EuroHPC Joint Undertaking , PRACE , EPI , ETP4HPC , EOSC , European Centre of Excellences (BioExcel, ChEESE, CompBioMed, E-cam, EoCoE, Esiwace, Excellerat,Hidalgo, Nomad, PerMedCoe, POP, Trex), FocusCoE, Psi-k, CECAM, Graphene Flagship, EMMC, Battery 2030, MMM - Materials and Molecular Modelling Hub.
Outline of engagement strategy	• Building long-term synergies with all the key players of the European HPC ecosystem through the organization of joint events. • Sharing MAX results with external stakeholders to share recommendations to be adopted for policy oriented documents. • Participating in 3rd-party and joint events organized by HPC players. • Co-organised events under the Focus CoE framework. • Publishing news and events on the dedicated sections on the MAX website. • Developing technical pages on the website focused on showing the MAX services, software, codes and data.

Table 2. Communication and dissemination activities towards the European institutions and ecosystem.

4.2 Industry

Industrial players are composed of commercial developers of materials simulation software (independent software vendors), industrial end users of materials modelling in small and large European companies, and hardware manufacturers and integrators. This SG generally lacks skills to use the MaX services and its ready-to-use codes and, for this reason, represents one of the main beneficiaries of the training offered by the project. The table below summarises the main benefits and strategy adopted to engage with them.

Description and Driver of the SG	**Community and Networks**
Short description of the SG	The Industry SG is composed of: • Independent software vendors (ISVs): broadly speaking, potential ISVs interested in MAX are companies operating in the broad materials, chemistry, pharmaceutical and biotechnology domain; • Industrial end users: it is composed of a wide spectrum of

	manufacturing companies (spanning from large, medium and small) covering several sectors and materials categories, from consumer goods to industrial chemicals, from polymers to alloys. The major driver for this SG lies in the usage of flagship codes and workflows, as well as in high level consulting and training; ● Hardware manufacturers and integrators (more detailed information on tangible collaborations with this SG have been reported and listed in the deliverable "D4.4 First report on co-design actions").
Benefits of cooperating with MAX	They are interested in using MAX open-source software and are interested in: ● Acquiring know-how in HPC architecture and software by joining the trainings organised by MAX; ● Supporting in codes development and consulting activities; ● Strengthening productive collaborations on co-design.
Sample of community	Simperler Consulting, P4BUS Systems, ATOS, Hexcel, Toyota Central R&D Labs. Inc. and Toyota Motor Europe, Synopsys Inc, Bright Computing, SUPERMICRO, ST Microelectronics, Vinformax, EXTOLL, ARM, Microsoft Research, Simune Atomistics, VASP Software Gmbh, Riken R-CCS, Umicore AG & Co. KG, Phasecraft Ltd, NVIDIA, Western Digital Technologies Inc., Clarivate Analytics, Tetra Pak, Samsung Electronics, Pintail Limited, Schott AG, SONY Europe Ltd, BIOVIA, Stratec BioMedical Romania SRL.
Outline of engagement strategy	● Participation in industry-oriented 3rd-party events. ● Focused training. ● Publication of news and events on the dedicated sections on the MAX website. ● Dedicated technical pages on the website focused on showing the MAX services, software, codes and data. ● MAX code webinars.

Table 3. Communication and dissemination activities towards industry.

4.3 Research and academia institutions

This SG includes research and academia institutions operating in the HPC and materials modelling ecosystems. The SG is interested in learning more about the research performed by MAX and contributes to its advancement through the release of new scientific publications. The table below summarises the main benefits and strategy put into place to achieve solid engagement.

Description and Driver of the SG	Community and Networks
Short description of the SG	Research and Academia institutions operating in the HPC and materials modelling ecosystems that might widely benefit from MAX freely accessible set of codes running optimally on a variety of platforms, and turn-key solutions that could allow them to calculate in-house the properties and performance of complex materials and devices.
Benefits of cooperating with MAX	They are interested in accessing ready-to-use codes and using them in turn-key solutions, as well as benefiting from support services.
Sample of community	ACM SIGHPC, AGH University of Science and Technology, Berlin Institute of Technology, Chalmers university of technology, EPFL Lausanne, Ghent University, ICHEC - Irish Centre for high end computing, Indian Institute of Information Technology, Institut de Quìmica Teorica i Computacional, JAMK University of Applied Sciences, KU Leuven, LMU Munich, Masaryk University, Newcastle University, NTNU, The University of Manchester, The University of Edinburgh, TU Delft - Delft University of Technology, Università di Milano, University of Twente, University of Zagreb - Faculty of electrical engineering and computing, UC3M Universidad Carlos III de Madrid, University of Luxembourg, University of Pisa, Utrecht University.
Outline of engagement strategy	• Outreach through publication of scientific papers, talks and posters. • Collecting user testimonials and stories for a well-grounded view of the benefits of MAX. • Training and schools organisation. • Attendance of scientific conferences. • Hackathons and technical workshops for flagship code users. • Contribution to implement teaching modules in Universities having Master/PhD programmes on Materials Science, HPC o computational modeling in their educational offer. • Organisation of events to promote the MAX main outputs. • Creation of sections on the website with the specific to share and put in the spotlight the scientific results of MAX (Science & MAX, publications).

Table 4. Communication and dissemination activities towards Research and academia institutions.

4.4 General public

This SG is composed of the general public who might be prevented from achieving a productive engagement with MAX due to the technical background required to understand the research topics developed by the project. However, one of the main goals of MAX is to involve as much as possible the general public to raise awareness and show the success of EU-funded initiatives and European collaborations. The table below summarises the main benefits and strategy adopted to engage with them.

Description and Driver of the SG	Community and Networks
Short description of the SG	This SG mainly refers to those lacking the necessary technical background and savviness in HPC and Materials Modeling, but nonetheless interested in increasing their average understanding of the HPC domain, as a whole. MAX Consortium envisaged a tailored and enhanced dissemination strategy towards societal end-users, with the purpose of introducing the general audience to materials modelling and the new exascale technology.
Benefits of cooperating with MAX	This SG is keen to learn about scientific and technological advances shaping tomorrow's society and economy from exascale to the development of innovative materials.
Outline of engagement strategy	● Creation of general and introductory pages about the project on the website that provide an easy and clear understanding of the MAX project. ● Development of a story-telling video[6] that shows how MAX creates ready-to-use solutions. ● Events organisation to share the project's results and key scientific outputs with a clear correlation to a societal impact. ● Direct interaction with the general public during public events such the European Researcher's Night.

Table 5. Communication and dissemination activities towards General public.

5. Communication and Dissemination impacts

The MAX communication partner, Trust-it has strictly cooperated with all partners, and especially with the leader node Cnr, in order to maximise the visibility and awareness of the project's main results and widely disseminate its outcomes and research findings. In particular, in order to achieve so, the CoE communication & dissemination

[6] MAX in a nutshell https://www.youtube.com/watch?v=do3Q68BibY0

policy focused on the following activities:

- Targeted messages to Stakeholder Groups (SGs);
- Implementation of SMART campaigns for social media channels (Specific, Measurable, Attainable, Relevant, and Timely);
- Revamp of the MAX website including new sections to better showcase the scientific contributions delivered in the projects' framework;
- Participation and organisation of events.

The impact of dissemination and communication activities was monitored throughout the entire lifespan of the project with defined KPIs, whose values are summarised in Section 5.8.

5.1 Website

At the launch of the project, the team designed and rolled out a new version of a fully operational website on Drupal, where the visitors can find general information and main results of the project, news and events connected to the HPC community, and dedicated pages for each of the MAX exascale codes. The new development started from the previous version of the MAX website (2015-2018 on Wordpress).

Over the lifespan of the project, the website went through two main revamps, at M11 and M26, that aimed to ensure a pleasant UX experience with enhanced visuals, new sections and pages that aim to streamline the communication and outreach for the MAX SGs.

Following thorough UX-based rules, the MAX team has gone through a series of fundamental steps, such as creating a draft version of the new website sections on a dedicated design tool called Figma and preparing a graphic mock-up, implementing the new section through technical programming and, finally, internal testing. The work required cross-disciplinary coordination moving through the Graphic, Technical and Marketing phases, as clearly outlined in the Figure below:

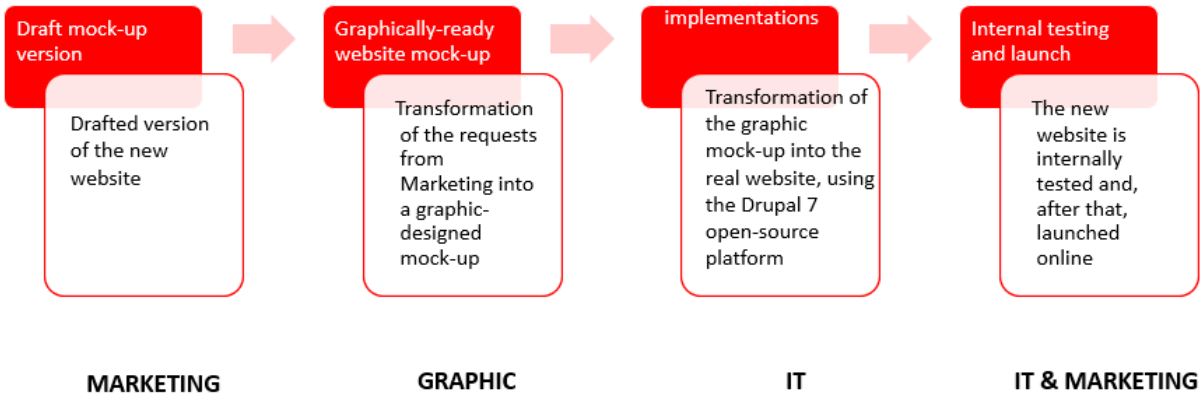


Figure 8. Process to design the MAX website revamps.

5.1.1 Website Iterations

The revamps of the website included the creation of new sections and significant improvements to already existing areas of the website. The paragraphs below show the main implemented changes.

About MAX

This section provides a clear and easy understanding of the overall concept of the project, as it contains sections dedicated to showing the project's goals, partners of the consortium, codes, project's repository, publications, job openings, newsletter, news and events. About MAX is the section of the website that allows a deeper involvement of the **general public**, thanks to the high-level information provided and easy content available.

Services

This section[7] is focused on delivering a competent user support and consulting services to serve the community of Research, Academia, and Industry. The offered services include Help Desk, MAX High level consultancy, Turn-key materials solutions, MAX Container technology for HPC system, Simulations on premises and in the cloud, Services to the Industry, and a FAQs area (dutifully described *at 3.3*).

Training

The Training[8] area comprises a wide range of freely accessible educational material produced under WP8 (Training and User Uptake) in the HPC and materials science domain for each exascale code. The training materials include the outcomes of online courses and schools, lectures, workshops, and webinars with a view to contribute to fill the sectoral skills gap. The Consortium gathered a collection of all the online events organized by MAX in 2021 in a dedicated Training Booklet, mainly focused on the theory, implementations, and use of the most used MAX flagship codes in the HPC environment (inclusive of freely accessible and browsable video lectures, slides and materials).

Facts and Figures

The sections Data, Services and Training includes tailored "Facts & Figures" that show in concise and eye-catching way the main outputs through visual infographics. Each "Facts & Figures" section is classified by year and shows the main achievements gained in the period 2019-2020, 2020-2021, and 2021-2022 (under development), and present the following sections:

- *Data Environment Facts & Figures*[9]
- *Services Facts & Figures*[10]
- *Training Facts & Figures*[11]

Frequently Asked Questions

The FAQs section[12] has been implemented to facilitate the research of answers to the most common issues linked to the flagship codes. This section helps the users in finding solutions to practical issues such as accounting problems, different environments or scheduler on different architectures.

Science & MAX

The new section was developed at the beginning of 2021 and aims to present the main achievements in terms of scientific research. In this section are featured both scientific papers that use or push forward the MAX flagship codes, written both by MAX scientists or by external authors if specially relevant.

[7] http://www.max-centre.eu/services
[8] http://www.max-centre.eu/training-and-education
[9] http://www.max-centre.eu/data/facts-figures
[10] http://www.max-centre.eu/services/facts-figures
[11] http://www.max-centre.eu/training/facts-figures
[12] http://www.max-centre.eu/services/faq

Science & MAX is staggered into 3 main sections:

- **Highlights**[13]: this area presents the papers in an appealing graphical manner, showing the journal in which the paper has been published, a snapshot image to sum up the work performed by the authors, the paper's abstract, authors' names, doi number and a short news about the publication (the latter is provided only for some papers, mainly authored by the MAX team).

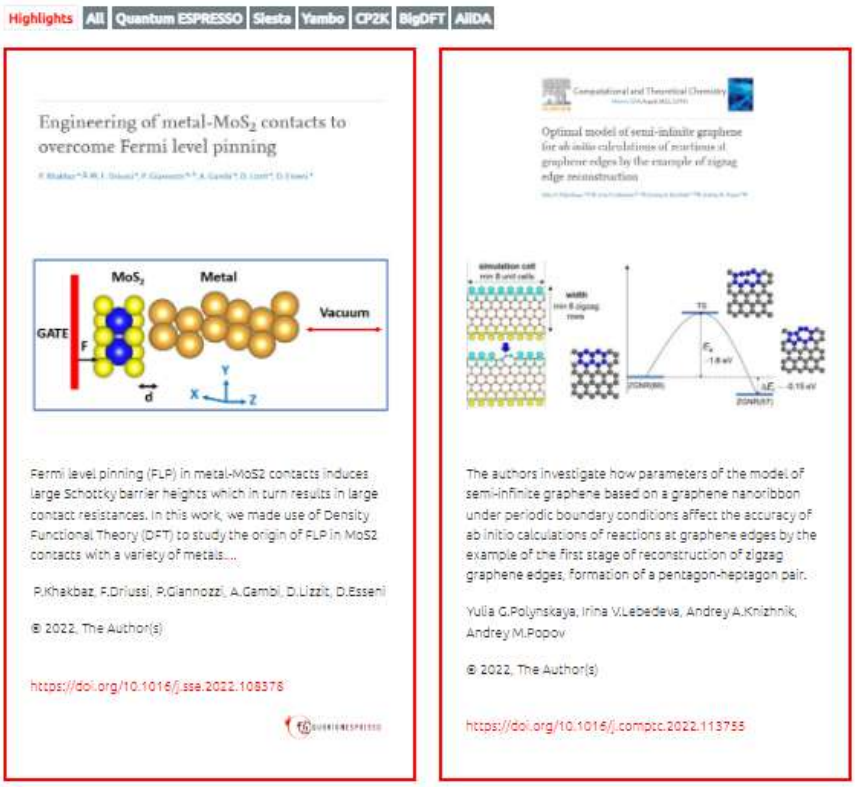


Figure 9. Printscreen of the Science & MAX - highlights section.

- **List of Publications**[14]: this area lists down the publications written by the MAX team and external authors that cite the MAX codes. The list shows the title, authors and DOI of the publications and the papers can be filtered by code.
- **Impact of MAX flagship codes**[15]: this section emphasizes the impact of the MaX flagship codes and geographical diffusion across the scientific community, viewable through maps collected. As for the publications, the Impact of MAX flagship codes can be filtered by code. The images below show some examples of the impacts generated by the flagship codes.

5.1.2 Website performances

MaX website proved to attain satisfactory web traffic throughout the lifespan of the project, as shown in the figures and tables below. The website performance is tracked on a dedicated website dashboard that allows a quicker analysis of the impact of data coming from Google Analytics. The main website achievements are

[13] http://www.max-centre.eu/science-and-max/highlights
[14] http://www.max-centre.eu/science-and-max
[15] http://www.max-centre.eu/impact-max-flagship-codes

summarized as it follows:

Website statistics. Critical figures to have a clear view of how many users access the website, unique users, page views, and the average engagement rate (how relevant the content is for them). More specifically, the quite low average bounce rate indicates how visitors usually engage in-depth with the website content, spending considerable time on each page and interacting with available links.

Website statistics	Value at Oct 2020 (mid-term of the project)	Value at Sept 2022 (end of the project)	Growth rate (Nov 2020 vs Sept 2022)
Number of unique users	29070	83200	186%
Number of sessions	40500	106100	162%
Number of pageviews	77148	180572	134%
Average bounce rate	69.85%	76.84%	10%

Table 6. Website statistics at M46.

The main achievements are summarised also in the graphics below.

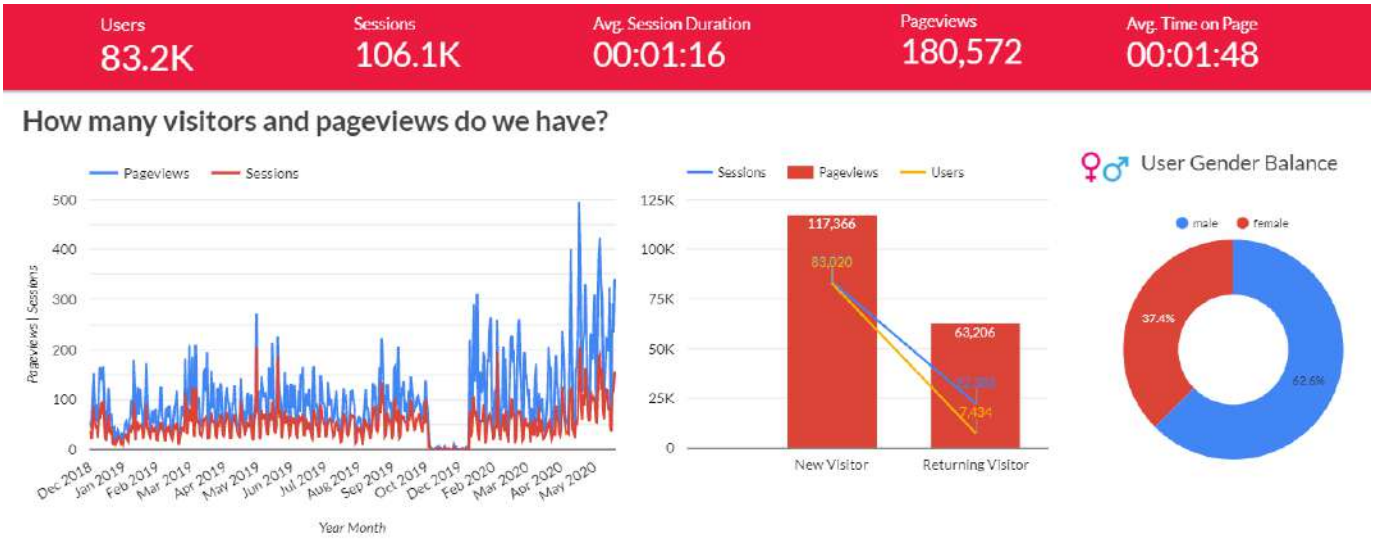
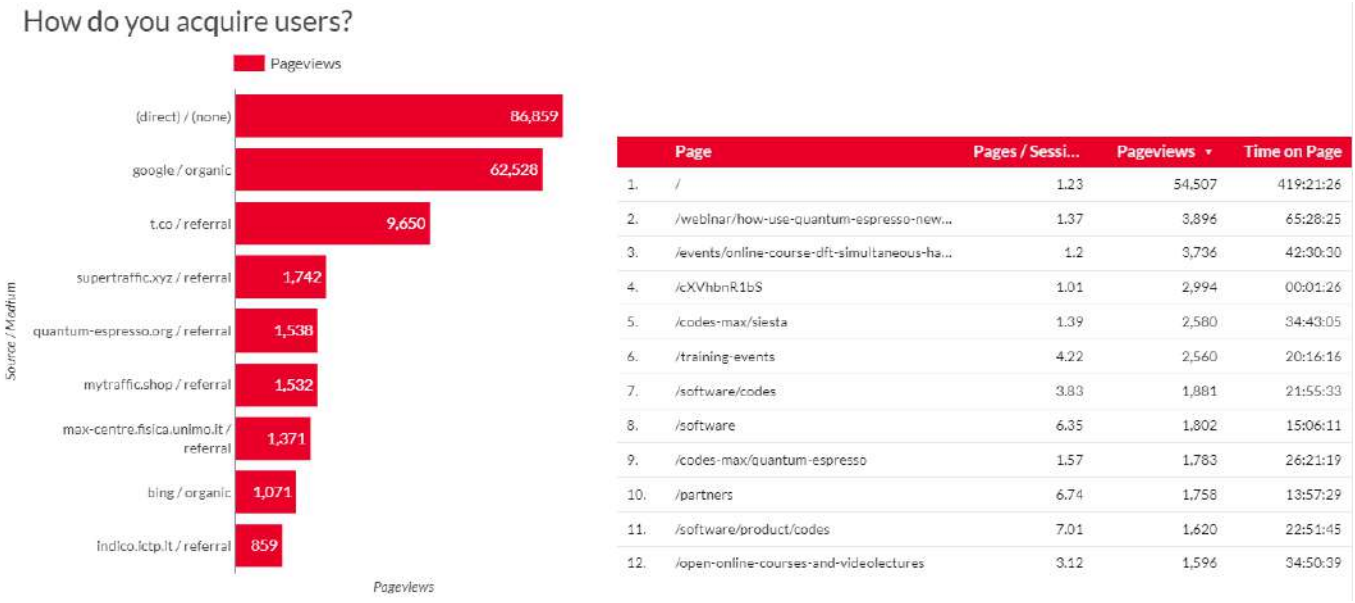


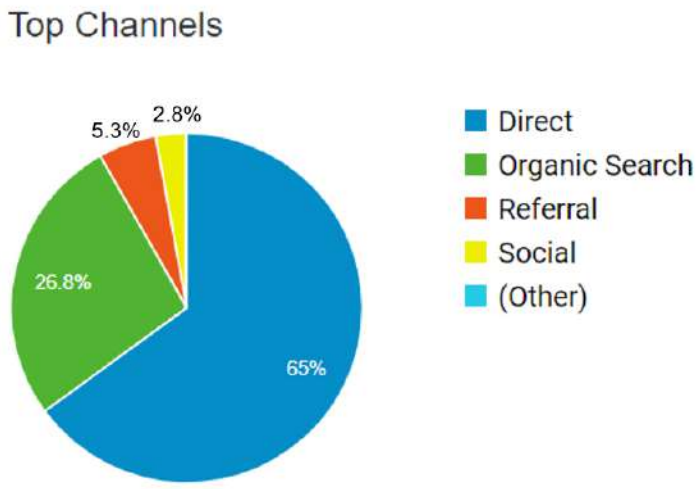
Figure 10. Dashboard: Website Statistics - Usage Data.



	Page	Pages / Sessi...	Pageviews ▾	Time on Page
1.	/	1.23	54,507	419:21:26
2.	/webinar/how-use-quantum-espresso-new...	1.37	3,896	65:28:25
3.	/events/online-course-dft-simultaneous-ha...	1.2	3,736	42:30:30
4.	/cXVhbnR1bS	1.01	2,994	00:01:26
5.	/codes-max/siesta	1.39	2,580	34:43:05
6.	/training-events	4.22	2,560	20:16:16
7.	/software/codes	3.83	1,881	21:55:33
8.	/software	6.35	1,802	15:06:11
9.	/codes-max/quantum-espresso	1.57	1,783	26:21:19
10.	/partners	6.74	1,758	13:57:29
11.	/software/product/codes	7.01	1,620	22:51:45
12.	/open-online-courses-and-videolectures	3.12	1,596	34:50:39

Figure 11. Dashboard: Website Statistics - Pageviews.

Website acquisition. Direct Access represents the main gateway to enter the website, meaning that the main part of users are "recurring users", people that already know the website URL and digit it directly on the main search engines to access the MAX website. Following that, the users visit the website through organic search. This value is quite high, showing that the website is well-ranked in terms of SEO for the most important key-terms. Referrals from external websites and social media are also productive traffic sources.



Countries. Website visitors mainly come from the United States, United Kingdom, Italy, and India. This is a very positive signal as, while the MAX activity is performed by European partners, the relevance and usefulness of the research is appreciated and leveraged by non-EU countries as well. The top 10 countries that visit the MAX are shown in the figure below.

Figure 12. Channels used to access the website.

	Country	Continent	Users
1.	United States	Americas	20.893
2.	United Kingdom	Europe	6.289
3.	Italy	Europe	6.024
4.	India	Asia	5.260
5.	Japan	Asia	3.368
6.	Germany	Europe	2.997
7.	Netherlands	Europe	2.742
8.	France	Europe	2.400
9.	China	Asia	2.379
10.	Finland	Europe	2.345
		Totale comples...	79.957

Figure 13. MAX Website traffic by country.

5.2 Social media channels

Social media are digital channels that have been used to consolidate the MAX online presence, communicate outputs, and engage with target SGs. The MAX channels used to serve this purpose are Twitter (@max_center2[16]) LinkedIn (@max-center[17]), and YouTube (@MaXCentreeXascale[18]). These channels are also used to run SMART campaigns that have specific launch, mid-term, and end dates to monitor performance throughout the entire lifespan. They are used to promote videos, webinars, workshops, training, MAX attendance at 3rd-party events to maximize outreach and impact through social media-driven communities, as well as promote publications or news of interest for the ecosystem.

Each social media channel fits into the communication strategy in a different way as described in the following paragraphs.

5.2.1 Twitter

Twitter is regularly used to provide real-time updates and news to promote events and takeaways, insights and results as the project matures. It is used to cover communication campaigns, such as events promotion, project's advancements, Twitter cards, to present the project's partners and their scientific standpoint on certain aspects of the project. Twitter proved to be a very effective platform to ensure a full coverage of live events through "live tweeting", with a view to provide timely updates and key takeaways for those unable to attend specific happenings. Finally, Twitter has been frequently leveraged to repurpose important materials and outputs over time, to maximise their exposure and enable accessibility and findability for the community. Some concrete examples are displayed below.

[16] https://twitter.com/max_center2
[17] https://www.linkedin.com/company/max-centre/
[18] https://www.youtube.com/c/MaXCentreeXascale/

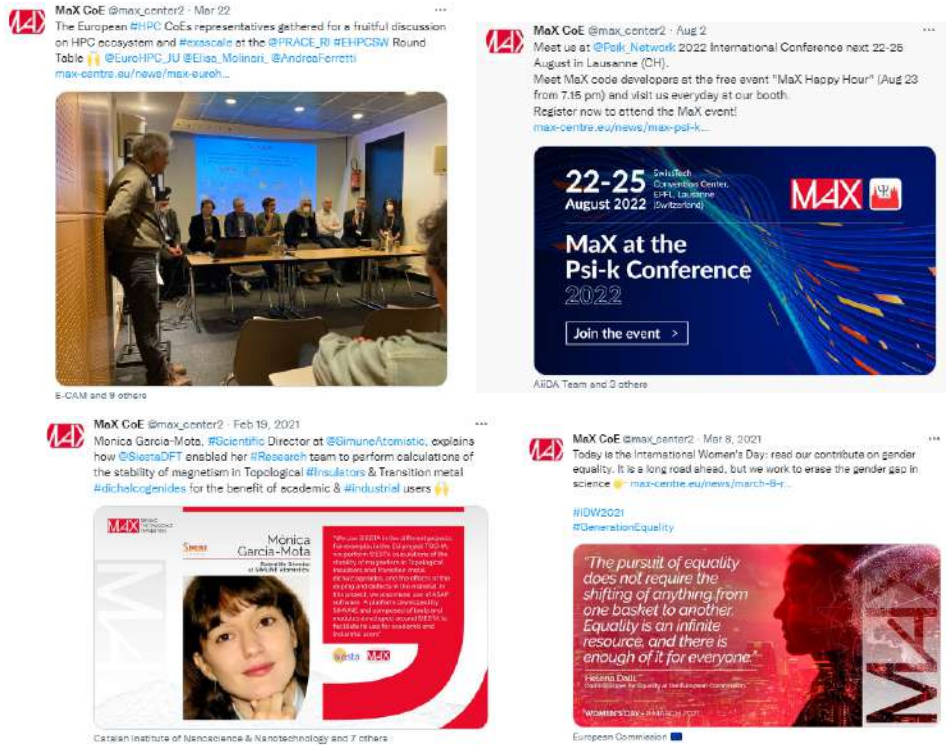


Figure 14. Examples of content released on Twitter.

Twitter's main achievements

- **1381 followers** garnering 1546 tweets, 7.1K likes, and 3.1K retweets;
- 65% growth in Twitter followers since M19 (June 2020).

Social Networks & Engagement

@max_center2

Followers count	1,381
Tweets count	1,546
Likes	7,026
Retweets	3,183

	Date	Link to tweet	Tweet	Likes	Retweets
1.	Sep 26, 2022	https://twitter.com/...	📣 @aiidateam Onli...	5	5
2.	Sep 19, 2022	https://twitter.com/...	📣 Trieste-Next: the ...	5	0
3.	Sep 19, 2022	https://twitter.com/...	Join the event:https:/...	0	0
4.	Sep 14, 2022	https://twitter.com/...	"Co-Design for #HP...	6	1
5.	Sep 12, 2022	https://twitter.com/...	Last day to register!...	5	2
6.	Sep 7, 2022	https://twitter.com/...	🎓 A post-doc posit!...	6	3
7.	Sep 5, 2022	https://twitter.com/...	The next hands-on tu...	5	1
8.	Sep 2, 2022	https://twitter.com/...	materials	0	0
9.	Aug 25, 2022	https://twitter.com/...	Thank you Patrick! It ...	4	1
10.	Aug 25, 2022	https://twitter.com/...	Merci merci! Thank y...	8	1

Figure 15. Dashboard: Twitter engagement.

5.2.2 LinkedIn

LinkedIn is mostly used to convey MAX advancements in terms of the project's main results across all the targeted stakeholder groups. It is also a primary source for building the community and for updating users about the main achievements of the project. One of the major benefits of LinkedIn is the possibility to obtain accurate community profiling, to reach out new members based on their professional roles and to connect with them. This has allowed MAX to build its network of core stakeholders. Examples of LinkedIn posts are given in the figure aside.

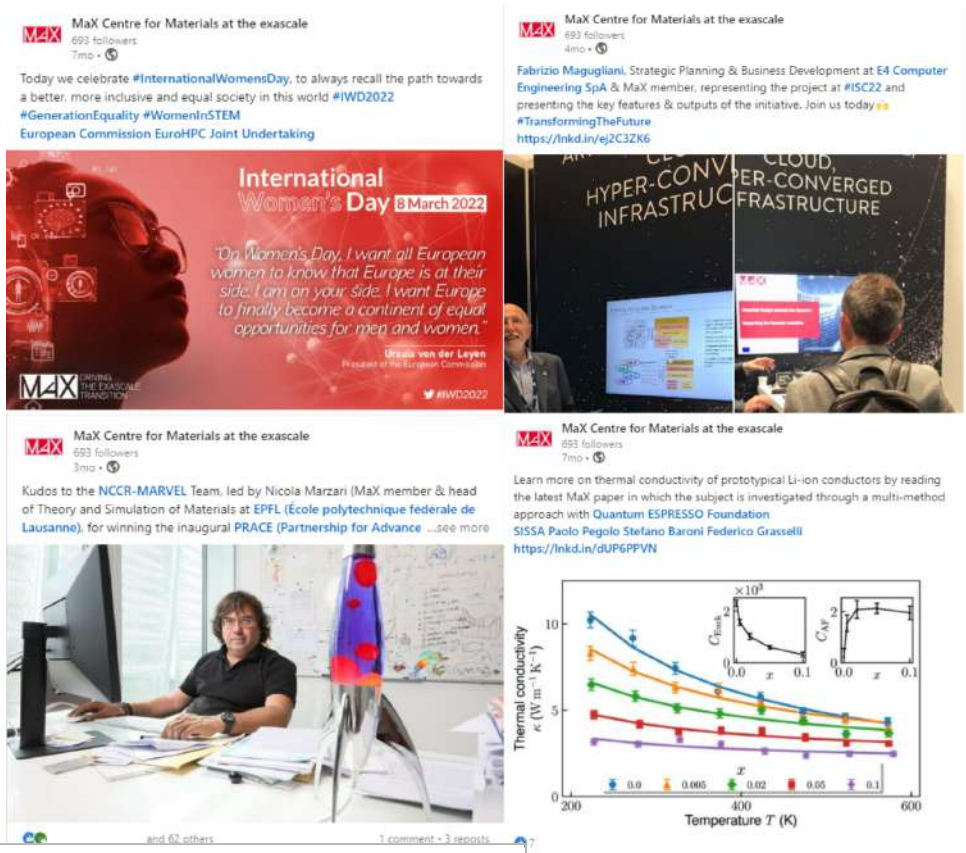


Figure 16. Examples of LinkedIn posts.

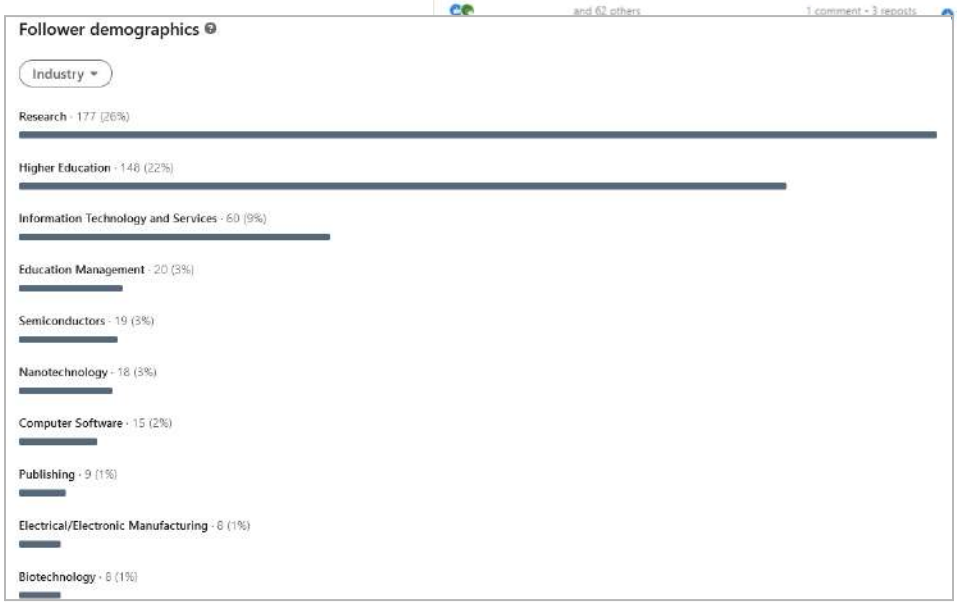


Figure 17. LinkedIn Followers' Demographics by Industry.

LinkedIn's main achievements

- **691 followers**, 305 posts and 718 likes.
- 189% growth in LinkedIn followers since M19 (June 2020).

The LinkedIn main achievements are also summarised in the image below.

	Date	Update content text	Likes	Engagements	Shares
1.	May 18, 20...	The Abdus Salam Internation...	14	172	1
2.	Sep 15, 2021	"Online course on Computati...	27	152	6
3.	Jun 22, 2022	Kudos to the NCCR-MARVE...	63	128	3
4.	Jun 20, 2022	The 7.1 version of Quantum ...	59	107	0
5.	Dec 22, 2021	Santa is coming and is bri...	29	71	0
6.	Sep 6, 2021	"Quantum ESPRESSO towar...	22	60	2
7.	Apr 15, 2022	Registration is open for Psi-k ...	20	59	0
8.	Dec 20, 2021	MaX is proud to present i...	13	54	3
9.	May 3, 2022	New file repository Simpl...	18	52	1
10.	Jan 31, 2022	A 5-day school of lectures &...	13	51	1

1 - 10 / 304

in/company/MaX Centre

Followers 691

Updates 305.0

Likes 718

Engagements 2.2K

Figure 18. Dashboard: LinkedIn engagement.

5.2.3 YouTube

Videos are an important asset to engage with the MAX targeted stakeholders and to deliver complex chunks of information into digestible content. The MAX videos, produced mostly by in-house specialists, are stored in a MAX YouTube channel that counts 155 videos, 14 playlists and 441 subscribers.

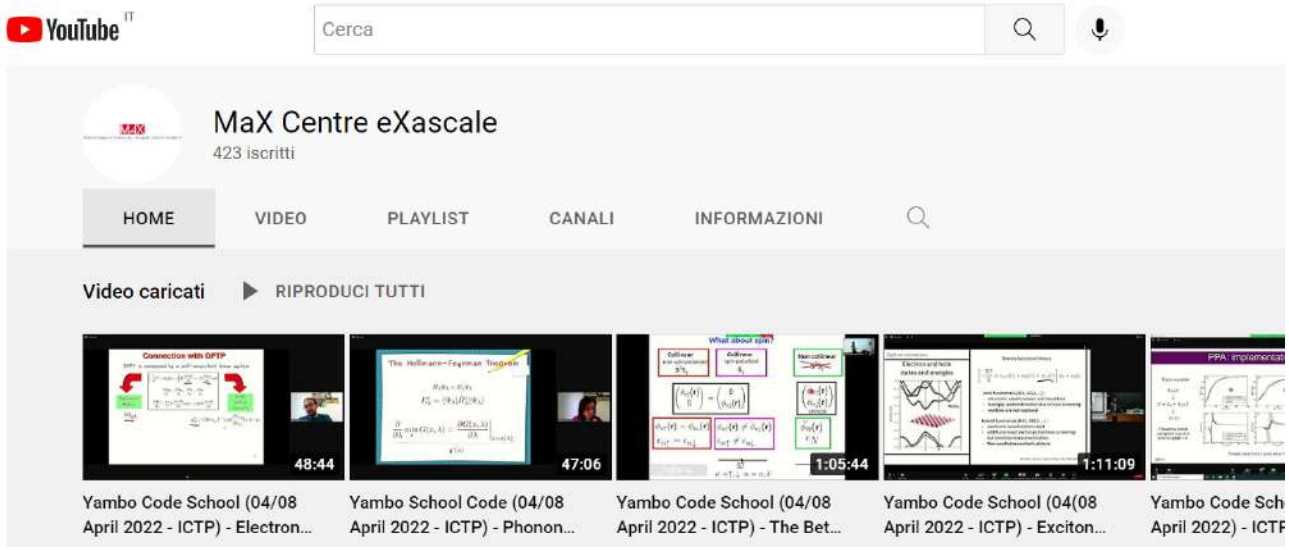


Figure 19. MAX YouTube channel Homepage.

The videos are either general ones that present the main objectives of the projects, recording of events organized and attended by the MAX team (like the webinar series on codes) and video lectures of training courses and schools.

5.3 Graphically-designed materials

A comprehensive overview of the project's Communication Kit, Visual Identity elements, and Graphics Collaterals have been provided in D9.1 and updated D9.3 (more examples of items publicly available in the website Communication area[19]). The rationale behind the harmonious development of this branding strategy was to reproduce a recognisable graphic pattern that could be reusable across multiple channels by the Consortium in its entirety and that could easily connect back to MAX.

Figure 20. Examples of graphic banners.

Another type of graphic material developed by the team was in the form of infographics and booklets. An example of highly-informative infographics are the Facts and Figures ones that show in a concise way the main outputs coming from the MAX Data, Services and Training, to provide an understandable overview to users.

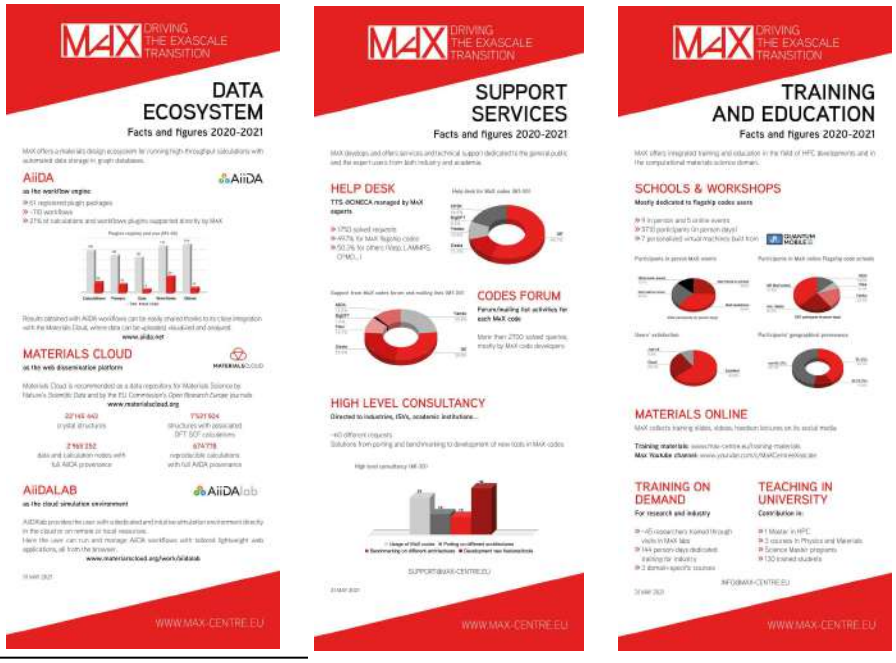


Figure 21. Screenshots of some MAX Facts and Figures sheets.

[19] http://www.max-centre.eu/communication

Educational booklets were also released to showcase the main results achieved from the organization of the MaX webinars and the school training. The booklets show in a compelling and intuitive way the main objectives of the events, the attendance rate, and the stakeholders engagement.

The booklets were published both in dedicated sections on the MAX website (**MAX webinars booklet**[20] / **MAX Training booklet**[21]) and uploaded on the project's Zenodo account to guarantee complete accessibility, in compliance with Open Access principles.

The booklets account at the moment of writing a total of 400+ visualizations, both on Zenodo and on the website.

Booklet name	Nr of visualizations on the website	Nr of visualizations on Zenodo	Nr of downloads on Zenodo
MAX webinars booklet	298	149	141
MAX training booklet	203	147	138

Table 7. KPIs of MAX booklets.

Figure 22. Pages from the MAX booklets.

Finally, in order to promote the MAX main achievements at the project final event (in conjunction with the Psi-K Conference, Lausanne, 22-25/08/2022), the team has also developed dedicated double-sided flyers, available both online[22] and in printed versions, to highlight the most innovative features and correlated case studies of each project's exascale codes.

[20] http://www.max-centre.eu/max-webinars-booklet
[21] http://www.max-centre.eu/max-training-booklet
[22] http://www.max-centre.eu/news/max-psi-k-conference

Figure 23. Some examples of the exascale code factsheets presented at the Psi-K conference.

5.4 Scientific publications

The research and development of the exascale codes by the MAX team contributes to the advancement of scientific investigation through the publication of scientific papers. The contribution of the MAX team in this area has been remarkable: the partners have published almost 100 papers in the last 30 months, some of which on leading journals, 16 of which concern the developments and advancements of the codes and the workflow.

The full list of scientific publications published in M19-46 is available in **Annex 2**.

5.5 Newsletter

Newsletters are a powerful tool to create or increase awareness, provide substantial information such as details of upcoming events and key insights from the past ones, or create a sense of stability and commitment for the project by sharing its achievements and relevant messages to the stakeholder's community. MaX has developed a branded newsletter with a stable framework to make it user friendly and entice the readers to take action. Over the entire timeframe of the project, 4 newsletters have been issued which have proved to be an effective way of engaging with the community, with an open rate > 30%. Currently, there are 859 subscribers.

Newsletter nr.	Date of delivery	Open rate	Clicks
1	April 2020	41.8%	9.9%
2	March 2022	40.1%	8.8%
3	August 2022	34.4%	3.9%
4	September 2022	55.3%	7.4%

Table 8. Newsletter performances.

5.6 Stakeholders Engagement events

As exhaustively described in precedent deliverables, MAX plan for stakeholder engagement needed to undergo a notable revision to timely and promptly face the unexpected Covid-19 pandemic side-effects, despite the organization or participation in a wide plethora of events, workshops, seminars, conferences, and trainings still sit at the core of the overall strategy. The collection of details on these events is done through a shared event tracker collecting all MAX-planned and attended events, by way of confirmed participation and/or (co-)organization, roles and related activities, including any papers submitted.

5.6.1 MaX training events, hackathons, schools and workshops

Training activities helped to widen the access to MAX codes and transfer the know-how to potential users. Given the crucial roles played by it, WP8 (Training and user uptake) and WP9 have closely worked together to deliver events aimed at increasing the skills in the HPC and material science fields for researchers, code users and student/developers.

In order to reach the majority of stakeholders, the training was organized in different formats: hackathons, schools, workshops, in-person and online lessons. Dedicated dissemination and communication activities were performed to increase the number of participants and awareness towards these events, like social media promotion, creation of training sections on the website and publication of the recording of the training on the MAX YouTube channel. All the materials produced are accessible in a dedicated section on the MAX website[23].

The complete list of training, hackathons and schools organized by the MAX team are presented in D8.3 and the main achievements gained by these outreach activities are listed as it follows:

- 21 of trainings organised by the MAX team;
- 1467 participants in training, schools, hackathons, workshops;
- Contributions to Master programmes (higher education) with introductory courses on computational materials science, hands-on sessions on usage of MAX flagship codes;
- 20 researchers hosted at MAX laboratories for basic and specialized training on MAX codes and libraries.

5.6.2 MaX webinars

The webinar series was organized over the course of 2020 by MaX and proved to be an effective way to update its users on the novelties introduced in the flagship codes which are being ported on these new conceptually different HPC systems, as well as to provide the community with valuable information on the actual deployment, usage and characteristics of the codes. The series was envisaged as a timely and prompt response to the ongoing pandemic wave that prevented the organization of the (originally planned) physical happenings and spanned from May to November 2020, driving a huge interest from the community and totalling the sizeable amount of nearly 950 participants from around 70 countries worldwide. A more detailed analysis, success stories, facts and figures and key takeaways of each webinar is dutifully encompassed and outlined in *D9.3 MAX Communication & Dissemination Strategy & Stakeholder Engagement Plan, Final version* (delivered in November 2020).

[23] http://www.max-centre.eu/training-materials

Finally, the main outcomes of the Webinar series have been gathered in a **dedicated Booklet**[24] (already anticipated and presented in section 5.3), freely available and downloadable for the community on Zenodo.

The main achievements gained by the webinar organisations are summarised in the table below.

Webinar title	Partners involved	Date	No. of attendees	Audience reached & Impacts achieved
Quasiparticle Band Structures and Excitons in Novel Materials using the **Yambo** Code	CNR, CINECA, Trust-IT	16/06/2020	185	**Audience**: Researchers, students and industries interested in Quasiparticle Band Structures and Excitons in Novel Materials. **Main impacts**: Social media campaign - May 2020/November 2020: 16.1K impressions on Twitter, 122 likes, 44 shares - Tweets most popular media (June 2020).
HPC libraries for **CP2K** and other electronic structure codes	ETH ZURICH, Trust-IT	24/06/2020	80	**Audience**: Researchers, scientists and industrial players interested in HPC libraries adopted by electronic structure codes. **Main impacts**: Social media campaign - May 2020/November 2020: 23K impressions on Twitter, 146 likes, 43 shares - Top Tweet and most popular mentions (June 2020).
New developments in **SIESTA** for high-performance materials simulations	ICN2, Trust-IT	22/09/2020	143	**Audience**: Researchers, scientists and students working in the HPC ecosystem and willing to discover more on the treatment of large systems with first-principles electronic-structure methods. **Main impacts**: Social media campaign - May 2020/November 2020: 37K impressions on Twitter, 209 likes, 81 shares - Top Tweet and most popular mentions (September 2020).
All-electron DFT using the **FLEUR** code	JUELICH, Trust-IT	14/10/2020	100	**Audience**: Researchers, Industrial and R&D end-users interested in all-electron full-potential linearised augmented plane-wave.

[24] https://zenodo.org/record/5109745#.Yv3mRC7P02w

				Main impacts: Social media campaign - May 2020/November 2020: 14K impressions, 93 likes, 25 shares - most popular mentions (October 2020).
The Flexibilities of Wavelets for Electronic Structure Calculations in Large Systems (**CP2K**)	CEA, Trust-IT	12/11/2020	73	**Audience**: Researchers and industry players involved in wavelets for electronic structure calculations in large systems. **Main impacts**: 13K impressions, 102 likes, 29 shares - Most popular Tweets, mentions (October 2020).

Table 9. Main impacts of MAX webinars (June-November 2020).

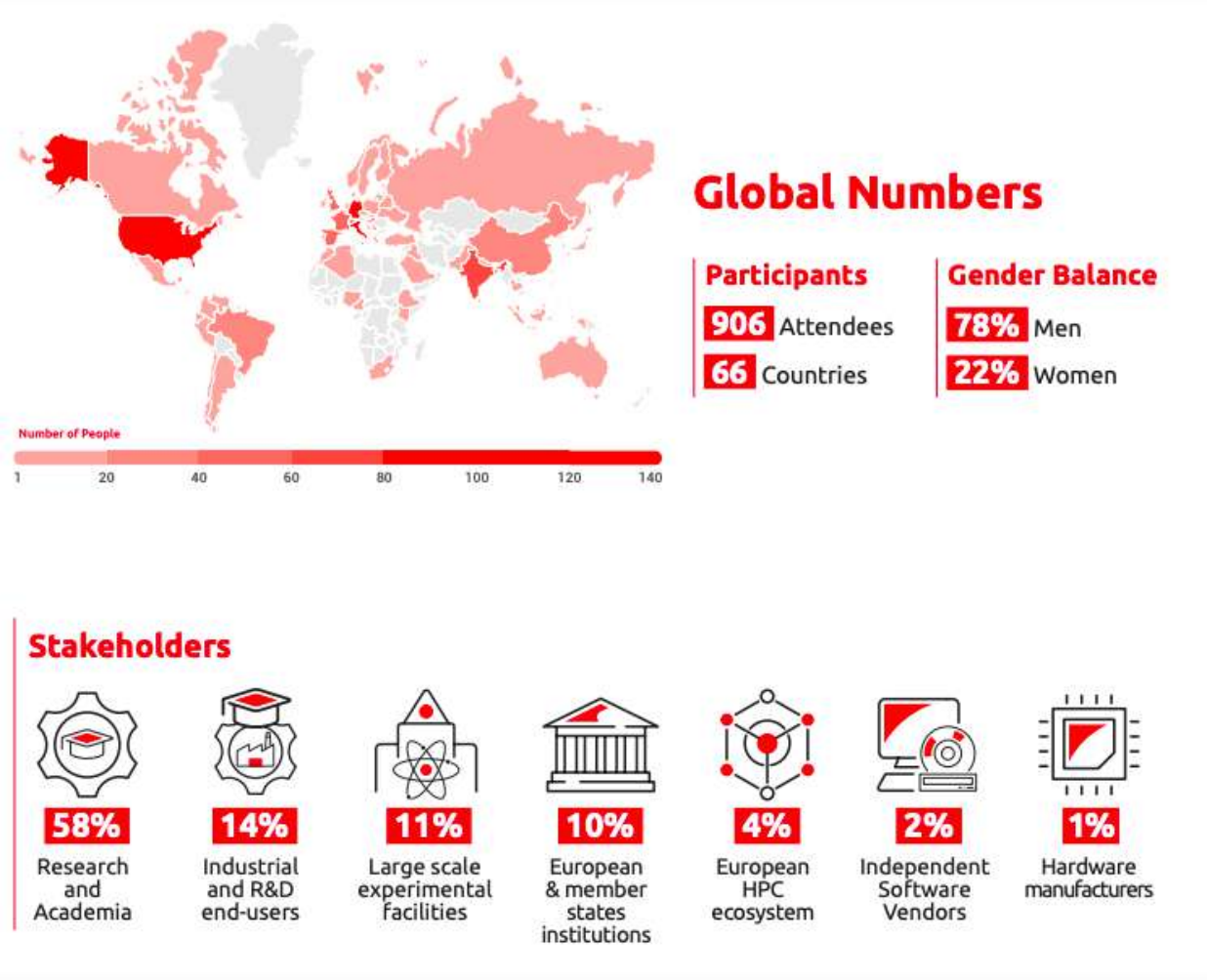


Figure 24. Global impact of the webinars (from the MAX webinar booklet).

5.6.3 Third-party events

Third-party events encompass workshops, conferences, coordination meetings, fairs and exhibitions, trainings and tutorials organized by external entities. The MAX consortium has joined more than 100 third-party events in these last months to keep updated with the latest discoveries in the HPC and material science environments and create engagement with the SGs identified in Section 4. Moreover, the attendance to third-party events helped the MAX team to raise awareness of the main achievements and advancements of MAX to an international community thanks to dedicated presentations held by project's partners.

The complete list of third-party events attended by the MAX team are shown in Annex 3. The events are classified by typology:

Category 1: presents scientific conferences and workshops on HPC, that target mostly the HPC community and HW stakeholders;

Category 2: shows scientific conferences and workshops in materials science and engineering, physics and chemistry, targeting mostly end-users of materials simulations in industry and academia, who are represented mainly by codes and ecosystem developers;

Category 3: showcases events aimed at engaging with the policy ecosystem;

Category 4: presents workshops and conferences that aim to train research and academia students;

Category 5: shows the 3rd-party events focused on outreach activities of the MAX main results.

5.7 KPI-driven approach and qualitative metrics

The impact of all strategically important WP9 activities performed are measured through a core set of key performance indicators (KPIs) wherever they are quantifiable. Qualitative metrics come into play whenever there is a need for a deeper analysis of the relevance of outcomes achieved.

The table below shows the end of project KPI targets and status at M46.

KPI	Target value	Achieved value in M46
Search Engine Optimization-driven website revamp tailored to MAX	Website revamp	Achieved
Website content-rich approach for the project entry point	Min. 1 content piece per week	Achieved
Community building on Twitter	Min 3 Tweets / week	Achieved - 1522 tweets
Community building on LinkedIn	Min 1 LinkedIn post / week	Achieved - 300 posts
Videos & YouTube Channel	Min. 1 project video/year for newcomers Min. 3 training promotional videos	Achieved Achieved

Collaterals and Promotional materials	KPIs: Min. 1 update every 6 months Min. 1 collaboration promotional pack/year Dedicated promotional packs for all events	Achieved Achieved Achieved
SlideShare or other platform	Dedicated dashboard connected to LinkedIn. KPIs: all training presentations clustered by stakeholders and topics. All presentations from technical and showcase events. Min. 1 updated project slide deck/year. Flash report monitoring on core statistics	N/A
Promotional campaigns on new documentation releases/guides	SMART-based campaign using a mix of the elements above.	Achieved
Training promotional campaigns	SMART-based campaign using a mix of the elements above.	Achieved

Table 10. Dissemination and Communication KPIs.

6. MaX @ Psi-K conference (Lausanne, August 22-25, 2022)

As from Task 9.4 in the DoA, MAX was committed to organize joint events with the community to maximize engagement and impact. To this aim, MAX participated in the Psi-K conference in Lausanne (August 22-25, 2022) by presenting several talks and posters and by organizing a special event, denominated "MAX Happy Hour". The Psi-K conference is usually organized every five years and this year it was held in person after a two year delay due to the pandemic. It is a major conference – the largest worldwide in electronic-structure – that brings together the community that is active in the field, as described by the Psi-K mission statement: "... to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours."[25]

It has been structured around 3.5 days, with 6 plenary talks, 38 symposia in 7 parallel sessions (114 invited talks and 252 contributed talks) and attended by 1250+ people. It was a great place to discuss the latest development in this scientific field, in code development, and in strengthening relations with the community.

MAX put a great effort in showcasing its activities and results at the conference, and participated with

- a booth
- 14 talks and 5 posters
- a special event "MAX Happy Hour"

A dedicated webpage in the MaX website was prepared for the event and is still available in the website[26]. Besides, MAX presence was backed up by an exhaustive Social Media coverage throughout the complete duration of the

[25] https://www.psik2020.net/
[26] http://www.max-centre.eu/news/max-psi-k-conference

event, to keep the large project's community updated on the main takeaways of the event, keynote speeches and talks and major appointments of the conference. Lastly, an extensive direct mail campaign was performed to reach out the project's SGs to promote the MAX special event and to gain the widest attention and participation.

6.1 MaX booth

Being one of the Silver Sponsors of the conference, MAX was given a booth in the main hall at the conference.

Figure 25. MAX booth @Psi-K 2022.

The booth was set up with fact-sheets about the latest achievements and outcomes of MAX and its flagship codes (see section 5.3 above), promotional materials about the network and its activities in training and services. Young developers from each code were available all the time to present the CoE and answer questions on the codes. Several people stopped by during the conference to meet our staff and to learn more about our activities, besides the booth soon turned into a meeting point for MAX people from all nodes, who had the chance of keeping up and discussing while attending the conference.

An additional MAX activity was shown at the nearby Lhumos booth. Lhumos is a training platform co-funded by MAX, Marvel and CECAM that is currently under development. It is designed to host all training materials prepared by the three groups, searchable by keywords, by level, that will permit different kinds of users to take advantage of all training materials developed in these years. It was presented at the conference and will soon be available online.

6.2 MAX Happy Hour

A dedicated event "MAX Happy Hour" took place on the Swiss Tech premises on Tuesday August 23 evening, after the end of the Conference session. It was conceived to make the MAX code developers meet with their main public, the users. Seven years after the Psi-K meeting in San Sebastian (ES, 2015), where MAX was first announced to the electronic structure community, in Lausanne the MaX partners had the chance of meeting the users of their flagship codes with the main goal of giving back to the community and discussing the status of electronic structure codes in a changing HPC landscape. The soiree was fully crowded and allowed us to meet in person with a large number of users and practitioners of electronic structure at HPC. After a first introductory report on the main achievements and challenges for the community, users had the opportunity to meet with the developers of each

MaX flagship code in a very friendly and informal event. Almost two hundred people attended the Happy Hour, after a long conference day, and gave us enthusiastic feedback about the event.

Figure 26. Scenes from the MAX Happy Hour @Psi-K 2022 (23/08/2022).

7. Conclusions

The D9.4 *MaX impact Assessment Report, Final Version* is the conclusive deliverable related to the *WP9 Engagement, Communication, Dissemination & Uptake*. The report summarizes the main achievements and impact generated in this area from M1 to M46 (extended lifespan of the project).

Given the collaborative nature of WP9, all partners and WPs of the project have contributed to the development of the MAX dissemination and communication actions, giving the consortium a well-acknowledged and recognised position in the relevant HPC and supercomputing related environments.

Thanks to this supportive approach and concerted action, over its lifetime, MAX has improved and strengthened its position in the European HPC ecosystem and gained a recognisable identity, spanning from enhancing the appeal of the

project website to the establishment of long-lasting synergies with other HPC CoEs in Europe and policy-oriented bodies, such as, e.g., HPC CoE Council (HPC3).

Several strategies were performed to increase the engagement level with identified stakeholders. One of these is linked to the organization of webinars and training, and participation in scientific conferences targeting mostly the HPC, industry, and policy communities, that helped to give visibility of the project and increase the basin of its stakeholder community. The project has also implemented a strong social media strategy to communicate to interested stakeholders the main achievements and advancements in terms of flagship codes development.

The implementation of new dissemination and communication strategy identified in D9.3 contributed to the consolidation of the MaX identity making the project recognisable, reliable and prominent in relevant areas, leaving a strong legacy and a wide (freely accessible) knowledge hub to tap into for the HPC research community.

ANNEX 1 - List of Acronyms

	Description
AiiDA	Automated Interactive Infrastructure and Database for computational science
CoE	Centre of Excellence
COVID-19	Coronavirus disease 2019
EU	European Union
FAQ	Frequently Asked Questions
HPC	High Performance Computing
HW	Hardware
KPI	Key Performance Indicator
MAX	Materials design at the eXascale
R&D	Research & Development
SG	Stakeholder Group
SMART	Specific, Measurable, Achievable, Realistic and Timed
UX Experience	User Experience
WP	Work Package

ANNEX 2 - List of scientific publications (all Open Access compliant)

CATEGORY 1: Scientific Publications targeting HPC community [HPC Centres]

1. *AiiDAlab -- an ecosystem for developing, executing, and sharing scientific workflows*, A. V. Yakutovich, K. Eimre, O. Schütt, L. Talirz, C. S. Adorf, C. W. Andersen, E. Ditler, D. Du, D. Passerone, B. Smit, N. Marzari, G. Pizzi, and C. A. Pignedoli, Computational Materials Science 188 (2021) DOI: 10.1016/j.commatsci.2020.110165

2. *AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance*, S. P. Huber, S. Zoupanos, M. Uhrin, L. Talirz, L. Kahle, R. Häuselmann, D. Gresch, T. Müller, A. V. Yakutovich, C. W. Andersen, F. F. Ramirez, C. S. Adorf, F. Gargiulo, S. Kumbhar, E. Passaro, C. Johnston, A. Merkys, A. Cepellotti, N. Mounet, N. Marzari, B. Kozinsky, and G. Pizzi, Sci Data 7, 300 (2020) DOI: 10.1038/s41597-020-00638-4

3. *Automated high-throughput Wannierisation*, V. Vitale, G. Pizzi, A. Marrazzo, J. Yates, N. Marzari, and A. Mostofi, npj Computational Materials 6, 66 (2020) DOI: 10.1038/s41524-020-0312-y

4. *Common workflows for computing material properties using different quantum engines*, S. P. Huber, E. Bosoni, M. Bercx, J. Bröder, A. Degomme, V. Dikan, K. Eimre, E. Flage-Larsen, A. Garcia, L. Genovese, D. Gresch, C. Johnston, G. Petretto, S. Poncé, G. Rignanese, C. J. Sewell, B. Smit, V. Tseplyaev, M. Uhrin, D. Wortmann, A. V. Yakutovich, A. Zadoks, P. Zarabadi-Poor, B. Zhu, N. Marzari, and G. Pizzi, npj Comput Mater 7, 136 (2021) DOI: 10.1038/s41524-021-00594-6

5. *Countdown Slack: A Run-Time Library to Reduce Energy Footprint in Large-Scale MPI Applications*, D. Cesarini, A. Bartolini, A. Borghesi, C. Cavazzoni, M. Luisier, and L. Benini, IEEE Transactions on Parallel and Distributed Systems, 31, 2696-2709 (2020) DOI: 10.1109/TPDS.2020.3000418

6. *ELSI -- An Open Infrastructure for Electronic Structure Solvers*, V. Wen-zhe Yu, C. Campos, W. Dawson, A. García, V. Havu, B. Hourahine, W. P Huhn, M. Jacquelin, W. Jia, M. Keçeli, R. Laasner, Y. Li, Lin Lin, J. Lu, J. Moussa, J. E Roman, Á. Vázquez-Mayagoitia, C. Yang, and V. Blum, Comp. Phys. Comm. Volume 256, 107459 (2020) DOI: 10.1016/j.cpc.2020.107459

7. *Materials Cloud, a platform for open computational science*, L. Talirz, I. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, M. Borelli, M. Uhrin, S. P. Huber, S. Zoupanos, C. S. Adorf, C. W. Andersen, O. Schütt, C. A. Pignedoli, D. Passerone, J. VandeVondele, T. C. Schulthess, B. Smit, G. Pizzi, and N. Marzari, Sci Data 7, 299 (2020) DOI: 10.1038/s41597-020-00637-5

8. *OPTIMADE: an API for exchanging materials data*, C. W. Andersen, R. Armiento, E. Blokhin, G. J. Conduit, S. Dwaraknath, M. L. Evans, A. Fekete, A. Gopakumar, S. Gražulis, A. Merkys, F. Mohamed, C. Oses, G. Pizzi, G. M. Rignanese, M. Scheidgen, L. Talirz, C. Toher, D. Winston, R. Aversa, K. Choudhary, P. Colinet, S. Curtarolo, D. Di Stefano, C. Draxl, S. Er, Suleyman;, M. Esters, M. Fornari, M. Giantomassi, M. Govoni, G. Hautier, V. Hegde, M. K. Horton, P. Huck, G. Huhs, J. Hummelshøj, A. Kariryaa, B. Kozinsky, S. Kumbhar, M. Liu, N. Marzari, A. J. Morris, A. Mostofi, K. A. Persson, G. Petretto, T. Purcell, F. Ricci, F. Rose, M. Scheffler, D. Speckhard, M. Uhrin, A. Vaitkus, P. Villars, D. Waroquiers, C. Wolverton, M. Wu, and X. Yang, Sci Data 8, 217 (2021) DOI: 10.1038/s41597-021-00974-z

9. *QEHeat: An open-source energy flux calculator for the computation of heat-transport coefficients from first*

principles, A. Marcolongo, R. Bertossa, D. Tisi, and S. Baroni, Computer Physics Communications 269, 108090 (2021) DOI: 10.1016/j.cpc.2021.108090

10. *SporTran: A code to estimate transport coefficients from the cepstral analysis of (multivariate) current time series*, L. Ercole, R. Bertossa, S. Bisacchi, and S. Baroni, Computer Physics Communications 280, 108470 (2022) DOI: 10.1016/j.cpc.2022.108470

11. *The CECAM Electronic Structure Library and the modular software development paradigm*, M. J. T. Oliveira, N. Papior, Y. Pouillon, V. Blum, E. Artacho, D. Caliste, F. Corsetti, S. de Gironcoli, A. M. Elena, A. Garcia, V. M. Garcia-Suarez, L. Genovese, W. P. Huhn, G. Huhs, S. Kokott, E. Kucukbenli, A. H. Larsen, A. Lazzaro, I. V. Lebedeva, Y. Li, D. Lopez-Duran, P. Lopez-Tarifa, M. Luders, M. A. L. Marques, J. Minar, S. Mohr, A. A. Mostofi, A. O'Cais, M. C. Payne, T. Ruh, D. G. A. Smith, J. M. Soler, D. A. Strubbe, N. Tancogne-Dejean, D. Tildesley, M. Torrent, and V. Wen-zhe Yu, J. Chem. Phys. 153, 024117 (2020) DOI: 10.1063/5.0012901

12. *turboMagnon – A code for the simulation of spin-wave spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation theory*, T. Gornia, O. Baseggio, P. Delugas, S. Baroni, and I. Timrov, Computer Physics Communication 280, 108500 (2022) DOI: 10.1016/j.cpc.2022.108500

13. *Unsupervised Learning Methods for Molecular Simulation Data*, A. Glielmo, B. E. Husic, A. Rodriguez, C. Clementi, F. Noé, and A. Laio, Chem. Rev. 121, 9722–9758 (2021) DOI: 10.1021/acs.chemrev.0c01195

14. *Virtual Computational Chemistry Teaching Laboratories—Hands-On at a Distance*, R. Kobayashi, T. P. M. Goumans, N. Ole Carstensen, T. Soini, N. Marzari, I. Timrov, S. Poncé, E. B. Linscott, C. J. Sewell, G. Pizzi, F. Ramirez, and M. Bercx, J. Chem. Educ. 98, 3163–3171 (2021) DOI: 10.1021/acs.jchemed.1c00655

15. *Workflow Engineering in Materials Design within the BATTERY 2030+ Project*, J. Schaarschmidt, J. Yuan, T. Strunk, I. Kondov, S. P. Huber, G. Pizzi, L. Kahle, F. T. Bölle, I. E. Castelli, T. Vegge, F. Hanke, T. Hickel, J. Neugebauer, C. R. C. Rêgo, and W. Wenzel, Advanced Energy Materials 12, 2102638 (2022) DOI: 10.1002/aenm.202102638

16. *Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows*, M. Uhrin, S. P. Huber, J. Yu, N. Marzari, and G. Pizzi, Computational Materials Science 187, 110086 (2020) DOI: 10.1016/j.commatsci.2020.110086

CATEGORY 2: Scientific Publications targeting end-users of materials simulations and code developers [codes and ecosystem developers]

17. *Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase*, S. Ossicini, I. Marri, M. Amato, M. Palummo, E. Canadell, and R. Rurali, Faraday Discuss. 222, 217 (2020) DOI: 10.1039/C9FD00085B

18. *Anomalous screening in narrow-gap carbon nanotubes*, G. Sesti, D. Varsano, E. Molinari, and M. Rontani, Phys. Rev. B 105, 195404 (2022) DOI: 10.1103/PhysRevB.105.195404

19. *Atomic-scale defects restricting structural superlubricity: Ab initio study study on the example of the twisted graphene bilayer*, A. S. Minkin, I. V. Lebedeva, A. M. Popov, and A. A. Knizhnik, Phys. Rev. B 104, 075444 (2021) DOI: 10.1103/PhysRevB.104.075444

20. *A Systematic Approach to Generating Accurate Neural Network Potentials: the Case of Carbon*, Y. Shaidu, E. Kucukbenli, R. Lot, F. Pellegrini, E. Kaxiras, and S. de Gironcoli, npj Computational Materials 7, 52 (2021) DOI: 10.1038/s41524-021-00508-6

21. *Basic aspects of the charge density wave instability of transition metal trichalcogenides NbSe3 and monoclinic-TaS3*, B. Guster, M. Pruneda, P. Ordejón, E. Canadell, and J.-P. Pouget, J. Phys.: Condens. Matter 33, 485401 (2021) DOI: 10.1088/1361-648X/ac238a

22. *Bulk and surface electronic structure of Bi4Te3 from GW calculations and photoemission experiments*, D. Nabok, M. Tas, S. Kusaka, E. Durgun, C. Friedrich, G. Bihlmayer, S. Blügel, T. Hirahara, and I. Aguilera, Phys. Rev. Materials 6, 034204 (2022) DOI: 10.1103/PhysRevMaterials.6.034204

23. *Coexistence of vortex arrays and surface capillary waves in spinning prolate superfluid 4 He nanodroplets*, M. Pi, J. M. Escartín, F. Ancilotto, and M. Barranco, Phys. Rev. B 104, 094509 (2021) DOI: 10.1103/PhysRevB.104.094509

24. *Coherence and de-coherence in the Time-Resolved ARPES of realistic materials: An ab-initio perspective*, A. Marini, E. Perfetto, and G. Stefanucci, Journal of Electron Spectroscopy and Related Phenomena 257, 147189 (2022) DOI: 10.1016/j.elspec.2022.147189

25. *Compact atomic descriptors enable accurate predictions via linear models*, C. Zeni, K. Rossi, A. Glielmo, and S. de Gironcoli, J. Chem. Phys. 154, 224112 (2021) DOI: 10.1063/5.0052961

26. *Competition between Ta-Ta and Te-Te bonding leading to the commensurate charge density wave in TaTe4*, B. Guster, M. Pruneda, P. Ordejón, and E. Canadell, Phys. Rev. B 105, 064107 (2022) DOI: 10.1103/PhysRevB.105.064107

27. *Data-driven simulation and characterisation of gold nanoparticle melting,* C. Zeni, K. Rossi, T. Pavloudis, J. Kioseoglou, S. de Gironcoli, R. E. Palmer, and F. Baletto, Nat Commun 12, 6056 (2021) DOI: 10.1038/s41467-021-26199-7

28. *Developing a Neural Network potential to investigate interface phenomena in solid-phase epitaxy*, R. Lot, L. Martin-Samos, S. De Gironcoli, and A. Hemeryck, 16th IEEE Nanotechnology Materials and Devices Conference, NMDC 2021 Vancouver proceedings (2021)

29. *Dynamic control of octahedral rotation in perovskites by defect engineering*, J. Jia, X. He, A. Akhtar, G. Herranz, and M. Pruneda, Phys. Rev. B 105, 224112 (2022) DOI: 10.1103/PhysRevB.105.224112

30. *Efficient hot-carrier dynamics in near-infrared photocatalytic metals*, C. E. P. Villegas, M. S. Leite, A. Marini, and A. R. Rocha, Phys. Rev. B 105, 165109 (2022) DOI: 10.1103/PhysRevB.105.165109

31. *Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method*, O. Motornyi, N. Vast, I. Timrov, O. Baseggio, S. Baroni, and A. Dal Corso, Physical Review B 102, 035156 (2020) DOI: 10.1103/PhysRevB.102.035156

32. *Electron–plasmon and electron–magnon scattering in ferromagnets from first principles by combining GW and GT self-energies*, D. Nabok, S. Blügel, and C. Friedrich, npj Computational Materials 7, 178 (2021) DOI: 10.1038/s41524-021-00649-8

33. *Electronic-structure methods for materials design*, N. Marzari, A. Ferretti, and C. Wolverton, Nature

Materials 20, 736 (2021) DOI: 10.1038/s41563-021-01013-3

34. *Electrosorption at metal surfaces from first principles*, N. G. Hörmann, N. Marzari, and K. Reuter, npj Computational Materials 6, 136 (2020) DOI: 10.1038/s41524-020-00394-4

35. *Engineering of metal-MoS2 contacts to overcome Fermi level pinning*, P. Khakbaz, F. Driussi, P. Giannozzi, A. Gambi D. Lizzit, and D. Esseni, Solid-State Electronics 194, 108378 (2022) DOI: 10.1016/j.sse.2022.108378

36. *Evidence for equilibrium exciton condensation in monolayer WTe2*, B. Sun, W. Zhao, T. Palomaki, Z. Fei, E. Runburg , P. Malinowski, X. Huang, J. Cenker, Y-T. Cui, J. Chu, X. Xu, S. Ataei, D. Varsano, M. Palummo, E. Molinari, M. Rontani, and D. H. Cobden, Nat. Phys. 18, 94 (2022) DOI: 10.1038/s41567-021-01427-5

37. *Evidence of ideal excitonic insulator in bulk MoS2 under pressure*, S. S. Ataei, D. Varsano, E. Molinari, and M. Rontani, PNAS March 30, 118 (2021) DOI: 10.1073/pnas.2010110118

38. *Exciton-Phonon Interaction and Relaxation Times from First Principles*, H. Chen, D. Sangalli, M. Bernardi, Phys. Rev. Lett. 125, 107401 (2020) DOI: 10.1103/PhysRevLett.125.107401

39. *Exciton-phonon interaction calls for a revision of the "exciton" concept,* F. Paleari and A. Marini, Phys. Rev. B 106, 125403 (2022), DOI: 10.1103/PhysRevB.106.125403

40. *Excitonic effects in graphene-like C3N*, M. Bonacci, M. Zanfrognini, E. Molinari, A. Ruini, M. J. Caldas, A. Ferretti, and D. Varsano, Phys. Rev. Materials 6, 034009 (2022) DOI: 10.1103/PhysRevMaterials.6.034009

41. *Excitons and carriers in transient absorption and time-resolved ARPES spectroscopy: An ab initio approach*, D. Sangalli, Phys. Rev. Materials 5, 083803 (2021) DOI: 10.1103/PhysRevMaterials.5.083803

42. *Exploring the robust extrapolation of high-dimensional machine learning potentials*, C. Zeni, A. Anelli, A. Glielmo, and K. Rossi, Phys. Rev. B 105, 165141 (2022) DOI: 10.1103/PhysRevB.105.165141

43. *Fast All-Electron Hybrid Functionals and Their Application to Rare-Earth Iron Garnets*, M. Redies, G. Michalicek, J. Bouaziz, C. Terboven, M. S. Müller, S. Blügel, and D. Wortmann, Front. Mater. 9, 851458 (2022) DOI: 10.3389/fmats.2022.851458

44. *Frequency dependence in GW made simple using a multi-pole approximation*, D.A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, and A. Ferretti, Phys. Rev. B 104, 115157 (2021) DOI: 10.1103/PhysRevB.104.115157

45. *Full orbital decomposition of Yu-Shiba-Rusinov states based on first principles*, T. G. Saunderson, J. F. Annett, G. Csire, and M. Gradhand, Phys. Rev. B 105, 014424 (2022) DOI: 10.1103/PhysRevB.105.014424

46. *Gap Opening in Double-Sided Highly Hydrogenated Free-Standing Graphene*, M. G. Betti, E. Placidi, C. Izzo, E. Blundo, A. Polimeni, M. Sbroscia, J. Avila, P. Dudin, K. Hu, Y. Ito, D. Prezzi, M. Bonacci, E. Molinari, and C. Mariani, Nano Lett. 22, 2971 (2022) DOI: 10.1021/acs.nanolett.2c00162

47. *Graphene decoupling through oxygen intercalation on Gr/Co and Gr/Co/Ir interfaces*, D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso, Phys. Rev. Materials 6, 064004 (2022) DOI: 10.1103/PhysRevMaterials.6.064004

48. *Halide Pb-free Double–Perovskites: Ternary vs. Quaternary Stoichiometry*, M. Palummo, D. Varsano, E.

Berríos, K. Yamashita, and G. Giorgi, Energies 13, 3516 (2020) DOI: 10.3390/en13143516

49. *Heat and charge transport in H2O at ice-giant conditions from ab initio MD simulations*, F. Grasselli, L. Stixrude, and S. Baroni, Nat Commun 11, 3605 (2020) DOI: 10.1038/s41467-020-17275-5

50. *Heat transport in liquid water from first-principles and deep-neural-network simulations*, D. Tisi, L. Zhang, R. Bertossa, H. Wang, R. Car, and S. Baroni, Phys. Rev. B 104, 224202 (2021) DOI: 10.1103/physrevb.104.224202

51. *Kerker mixing scheme for self-consistent muffin-tin based all-electron electronic structure calculations*, M. Winkelmann, E. Di Napoli, D. Wortmann, and S. Blügel, Phys. Rev. B 102, 195138 (2020) DOI: 10.1103/PhysRevB.102.195138

52. *Interference effects in one-dimensional moiré crystals*, N. Wittemeier, M. J. Verstraete, P. Ordejón, and Z. Zanolli, Carbon 186, 416 (2022) DOI: 10.1016/j.carbon.2021.10.028

53. *Invariance principles in the theory and computation of transport coefficients*, F. Grasselli and S. Baroni, Eur. Phys. J. B 94, 160 (2021) DOI: 10.1140/epjb/s10051-021-00152-5

54. *Large Dzyaloshinskii-Moriya interaction induced by chemisorbed oxygen on a ferromagnet surface*, G. Chen, A. Mascaraque, H. Jia, B. Zimmermann, M.C. Robertson, R. Lo Conte, M. Hoffmann, M. A. González Barrio, H. Ding, R. Wiesendanger, E. G. Michel, S. Blügel, A. K. Schmid, and K. Liu, Science Advances 6, 33 (2020) DOI: 10.1126/sciadv.aba4924

55. *Localized electronic vacancy level and its effect on the properties of doped manganites*, D. Juan, M. Pruneda, and V. Ferrari, Scientific Reports 11, 6706 (2021) DOI: 10.1038/s41598-021-85945-5

56. *Magnetic properties of coordination clusters with {Mn4} and {Co4} antiferromagnetic cores*, S. Achilli, C. Besson, X. He, P. Ordejón, C. Meyer, and Z. Zanolli, Phys. Chem. Chem. Phys. 24, 3780 (2022) DOI: 10.1039/D1CP03904K

57. *Magnetic response and electronic states of well defined Graphene/Fe/Ir(111) heterostructure*, C. Cardoso, G. Avvisati, P. Gargiani, M. Sbroscia, M. S. Jagadeesh, C. Mariani, D. A. Leon, D. Varsano, A. Ferretti, and M. G. Betti, Phys. Rev. Materials 5, 014405 (2021) DOI: 10.1103/PhysRevMaterials.5.014405

58. *Manipulation of spin transport in graphene/transition metal dichalcogenide heterobilayers upon twisting*, A. Pezo, Z. Zanolli, N. Wittemeier, P. Ordejon, A. Fazzio, S. Roche, and J. H. Garcia, 2D Mater. 9, 015008 (2021) DOI: 10.1088/2053-1583/ac3378

59. *Material systems for FM-/AFM-coupled skyrmions in Co/Pt-based multilayers*, H. Jia, B. Zimmermann, M. Hoffmann, M. Sallermann, G. Bihlmayer, and S. Blügel, Phys. Rev. Materials 4, 094407 (2020) DOI: 10.1103/PhysRevMaterials.4.094407

60. *Measuring shared electrons in extended molecular systems: Covalent bonds from plane-wave representation of wave function*, G. La Penna, D. Tiana, and P. Giannozzi, Molecules 26, 131, 4044 (2021) DOI: 10.3390/molecules26134044

61. *Merging of superfluid helium nanodroplets with vortices*, J. M. Escartín, F. Ancilotto, M. Barranco, and M. Pi, Phys. Rev. B 105, 024511 (2022) DOI: 10.1103/PhysRevB.105.024511

62. *Microscopic picture of paraelectric perovskites from structural prototypes*, M. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, and G. Pizzi, Phys. Rev. Research 4, L012042 (2022) DOI: 10.1103/PhysRevResearch.4.L012042

63. *Multiple exciton generation in isolated and interacting silicon nanocrystals*, I. Marri and S. Ossicini, Nanoscale 13, 12119-12142 (2021) DOI: 10.1039/D1NR01747K

64. *Multiscale modeling strategy to solve fullerene formation mystery*, A. M. Popov, I. V. Lebedeva, S. A. Vyrko, and N. A. Poklonski, Fullerenes Nanotubes and Carbon Nanostructures 29, 755 (2021) DOI: 10.1080/1536383X.2021.1900124

65. *Narrowing of d bands of FeCo layers intercalated under graphene*, D. Pacilè, C. Cardoso, G. Avvisati, I. Vobornik, C. Mariani, D. A. Leon, P. Bonfà, D. Varsano, A. Ferretti, and M. G. Betti, Appl. Phys. Lett. 118, 121602 (2021) DOI: 10.1063/5.0047266

66. *Numerically Precise Benchmark of Many-Body Self-Energies on Spherical Atoms*, S. Vacondio, D. Varsano, A. Ruini, and A. Ferretti, J. Chem. Theory Comput. 2022, 18, 6, 3703–3717 (2022) DOI: 10.1021/acs.jctc.2c00048

67. *Observation of an Excitonic Mott Transition through Ultrafast Core-cum-Conduction Photoemission Spectroscopy*, M. Dendzik, R. P. Xian, E. Perfetto, D. Sangalli, D. Kutnyakhov, S. Dong, S. Beaulieu, T. Pincelli, F. Pressacco, D. Curcio, S. Y. Agustsson, M. Heber, J. Hauer, W. Wurth, G. Brenner, Y. Acremann, P. Hofmann, M. Wolf, A. Marini, G. Stefanucci, L. Rettig, and R. Ernstorfer, Phys. Rev. Lett. 125, 096401 (2020) DOI: 10.1103/PhysRevLett.125.096401

68. *Optical Signatures of Defect Centres in Transition Metal Dichalcogenide Monolayers*, P. M. M. C. de Melo, Z. Zanolli, and M. J. Verstraete, Advanced Quantum Technologies (2021) DOI: 10.1002/qute.202000118

69. *Oxidation states, Thouless' pumps, and anomalous transport in non-stoichiometric ionic conductors*, P. Pegolo, F. Grasselli, and S. Baroni, Phys. Rev. X 10, 041031 (2020) DOI: 10.1103/PhysRevX.10.041031

70. *Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory*, F. Libbi, P. M. M. C. de Melo, Z. Zanolli, M. J. Verstraete, and N. Marzari, Phys. Rev. Lett. 128, 167401 (2022) DOI: 10.1103/PhysRevLett.128.167401

71. *Photoinduced modulation of the excitonic resonance via coupling with coherent phonons in a layered semiconductor*, S. Mor, V. Gosetti, A. Molina-Sánchez, D. Sangalli, S. Achilli, V. F. Agekyan, P. Franceschini, C. Giannetti, L. Sangaletti, and S. Pagliara, Phys. Rev. Research 3, 043175 (2021), DOI: 10.1103/PhysRevResearch.3.043175

72. *Prediction of Phonon-Mediated Superconductivity with High Critical Temperature in the Two-Dimensional Topological Semimetal W2N3*, D. Campi, S. Kumari, and N. Marzari, Nano Lett. 21, 3425 (2021) DOI: 10.1021/acs.nanolett.0c05125

73. *Proximity effect in a superconductor–topological insulator heterostructure based on first principles*, K.Park, G. Csire, and B. Ujfalussy, Phys. Rev. B 102, 134504 (2020) DOI: PhysRevB.102.134504

74. *Ranking the information content of distance measures*, A. Glielmo, C. Zeni, B. Cheng, G. Csányi, and A. Laio,

PNAS Nexus, pgac039 (2022) DOI: 10.1093/pnasnexus/pgac039

75. *Real-space multiple scattering theory for superconductors with impurities*, T. G. Saunderson, Z. Győrgypál, J. F. Annett, G. Csire, B. Újfalussy, and M. Gradhand, Physical Review B 102, 245106 (2020) DOI: 10.1103/PhysRevB.102.245106

76. *Real-time modelling of Optical orientation in GaAs: generation and decay of the degree of spin polarization*, M. D'Alessandro and D. Sangalli, Phys. Rev. B 102, 104437 (2020) DOI: 10.1103/PhysRevB.102.104437

77. *Relativistic first-principles theory of Yu-Shiba-Rusinov states applied to Mn adatoms and Mn dimers on Nb(110)*, B. Nyári, A. Lászlóffy, L. Szunyogh, G. Csire, K. Park, and B. Ujfalussy, Phys. Rev. B 104, 235426 (2021), DOI: 10.1103/PhysRevB.104.235426

78. *Self-consistent screening enhances stability of the nonequilibrium excitonic insulator phase*, E. Perfetto, A. Marini, G. Stefanucci, Phys. Rev. B 102, 085203 (2020) DOI: 10.1103/PhysRevB.102.085203

79. *Shear and breathing modes of layered materials*, G. Pizzi, S. Milana, A. C. Ferrari, N. Marzari, and M. Gibertini, ACS Nano 15, 12509–12534 (2021) DOI: 10.1021/acsnano.0c10672

80. *Solution to the Modified Helmholtz Equation for Arbitrary Periodic Charge Densities*, M. Winkelmann, E. Di Napoli, D. Wortmann, and S. Blügel, Front. Phys. 8, 618142 (2021) DOI: 10.3389/fphy.2020.618142

81. *Spinorial formulation of the GW -BSE equations and spin properties of excitons in two-dimensional transition metal dichalcogenides*, M. Marsili, A. Molina-Sánchez, M. Palummo, D. Sangalli, and A. Marini, Phys. Rev. B 103, 155152 (2021) DOI: 10.1103/PhysRevB.103.155152

82. *Structural and magnetic phase diagram of epitaxial* $La_{0.7}Sr_{0.3}Mn_{O3}$ *from first principles*, J. Pilo, M. Pruneda, and N. C. Bristowe, Electron. Struct. 3, 024001 (2021) DOI: 10.1088/2516-1075/abe6af

83. *Subpicosecond metamagnetic phase transition driven by non-equilibrium electron dynamics*, F. Pressacco, D. Sangalli, V. Uhlíř, D. Kutnyakhov, J. A. Arregi, S. Y. Agustsson, G. Brenner, H. Redlin, M. Heber, D. Vasilyev, J. Demsar, G. Schönhense, M. Gatti, A. Marini, W. Wurth, and F.Sirotti, Nature Communications 12, 5088 (2021) DOI: 10.1038/s41467-021-25347-3

84. *Surface chemistry effects on work function, ionization potential and electronic affinity of Si(100), Ge(100) surfaces and SiGe heterostructures*, I. Marri, M. Amato, M. Bertocchi, A. Ferretti, D. Varsano, and S. Ossicini, Phys. Chem. Chem. Phys. 22, 25593-25605 (2020) DOI: 10.1039/D0CP04013D

85. *Surface termination dependence of electronic and optical properties in Ti2CO2 MXene monolayers*, Z. Kandemir, E. Torun, F. Paleari, C. Yelgel, and C. Sevik, Phys. Rev. Materials 6, 026001 (2022) DOI: 10.1103/PhysRevMaterials.6.026001

86. *Temperature- and vacancy-concentration-dependence of heat transport in Li3ClO from multi-method numerical simulations*, P. Pegolo, S. Baroni, and F. Grasselli, npj Comput Mater 8, 24 (2022) DOI: 10.1038/s41524-021-00693-4

87. *Thermal and Tidal Evolution of Uranus with a Growing Frozen Core*, L. Stixrude, S. Baroni, and F. Grasselli, Planet. Sci. J. 2, 222 (2021) DOI: 10.3847/PSJ/ac2a47

88. *Time-dependent screening explains the ultrafast excitonic signal rise in 2D semiconductors*, V. Smejkal, F. Libisch, A. Molina-Sanchez, L. Wirtz, and A. Marini, ACS Nano 15, 1179–1185 (2021) DOI: 10.1021/acsnano.0c08173

89. *Topology, Oxidation States, and Charge Transport in Ionic Conductors*, P. Pegolo, S. Baroni, and F. Grasselli, Annalen der physik 2200123 (2022) DOI: 10.1002/andp.202200123

90. *Tuning the topological band gap of bismuthene with silicon-based substrates*, N. Wittemeier, P. Ordejón, and Z. Zanolli, J. Phys. Mater. 5, 035002 (2022) DOI: 10.1088/2515-7639/ac84ad

91. *Unified Green's function approach for spectral and thermodynamic properties from algorithmic inversion of dynamical potentials*, T. Chiarotti, N. Marzari, and A. Ferretti, Phys. Rev. Research 4, 013242 (2022) DOI: 10.1103/PhysRevResearch.4.013242

92. *Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application*, M. G. Pala, P. Giannozzi, and D. Esseni, Phys. Rev. B 102, 045410 (2020) DOI: 10.1103/PhysRevB.102.045410

93. *Unraveling Heat Transport and Dissipation in Suspended MoSe2 from Bulk to Monolayer*, D. Saleta Reig, S. Varghese, R. Farris, A. Block, J. D. Mehew, O. Hellman, P. Woźniak, M. Sledzinska, A. El Sachat, E. Chávez-Ángel, S. O. Valenzuela, N. F. van Hulst, P. Ordejón, Z. Zanolli, C. M. Sotomayor Torres, M. J. Verstraete, and K.-J. Tielrooij, Adv. Mater. 2108352 (2022) DOI: 10.1002/adma.202108352

94. *Validity of the on-site spin-orbit coupling approximation*, R. Cuadrado, R. Robles, A. García, M. Pruneda, P. Ordejón, J. Ferrer, and J. I. Cerdá, Phys. Rev. B 104, 195104 (2021) DOI: 10.1103/PhysRevB.104.195104

95. *Vibrational signature of the graphene nanoribbon edge structure from high-resolution electron energy-loss spectroscopy*, N. Cavani, M. De Corato, A. Ruini, D. Prezzi, E. Molinari, A. Lodi Rizzini, A. Rosi, R. Biagi, V. Corradini, X.-Y. Wang, X. Feng, A. Narita, K. Muellen, and V. De Renzi, Nanoscale 12, 19681-19688 (2020) DOI: 10.1039/D0NR05763K

96. *Viscosity in water from first-principles and deep-neural-network simulations*, C. Malosso, L. Zhang, R. Car, S. Baroni, and D. Tisi, npj Comput Mater 8, 139 (2022) DOI: 10.1038/s41524-022-00830-7

Preprint papers

97. *Magnon-phonon interactions open a gap at the Dirac point in the spin-wave spectra of CrI3 2D magnets*, P. Delugas, O. Baseggio, I. Timrov, S. Baroni, and T. Gorni, https://arxiv.org/abs/2105.04531

98. *Modular implementation of linear and cubic-scaling approaches based on the orbital minimization method in electronic structure codes using atomic orbitals*, I. V. Lebedeva, A.Garcıa, E. Artacho, and P. Ordejon, https://arxiv.org/abs/2209.05934

Papers published in the first reporting period (not inserted in the previous deliverable D 9.2)

99. *Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding*, W. Dawson, S. Mohr, L. E. Ratcliff, T. Nakajima, and L. Genovese, J. Chem. Theory Comput. 16, 2952–2964 (2020), DOI: 10.1021/acs.jctc.9b01152

100. *CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations*, T.D. Kühne, M. Iannuzzi, M. Del Ben, V.V. Rybkin, P. Seewald, F. Stein, T.

Laino, R. Z. Khaliullin, O. Schütt, F. Schiffmann, D. Golze, J. Wilhelm, S. Chulkov, M. Hossein Bani-Hashemian, V. Weber, U. Borštnik, M. Taillefumier, A.S. Jakobovits, A. Lazzaro, H. Pabst, T. Müller, R. Schade, M. Guidon, S. Andermatt, N. Holmberg, G. K. Schenter, A. Hehn, A. Bussy, F. Belleflamme, G. Tabacchi, A. Glöß, M. Lass, I. Bethune, C.J. Mundy, C. Plessl, M. Watkins, J. VandeVondele, M. Krack, and J. Hutter, J. Chem. Phys. 152, 194103 (2020) DOI: 10.1063/5.0007045

101. *Emergent dual topology in the three-dimensional Kane-Mele Pt2HgSe3*, A. Marrazzo, N. Marzari, and M. Gibertini, Physical Review Research 2, 012063 (2020) DOI: 10.1103/PhysRevResearch.2.012063

102. *Equipartition of Energy Defines the Size− Thickness Relationship in Liquid-Exfoliated Nanosheets*, C. Backes, D. Campi, B. M. Szydłowska, K. Synnatschke, E. Ojala, F. Rashvand, A. Harvey, A. Griffin, Z. Sofer, N. Marzari, J. N. Coleman, and D. D. O'Regan, ACS Nano 13, 7050−7061 (2019) DOI: 10.1021/acsnano.9b02234

103. *Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations*, L. E. Ratcliff, W. Dawson, G. Fisicaro, D. Caliste, S. Mohr, A. Degomme, B. Videau, V. Cristiglio, M. Stella, M. D'Alessandro, S. Goedecker, T. Nakajima, T. Deutsch, and L. Genovese, J. Chem. Phys. 152, 194110 (2020) DOI: 10.1063/5.0004792

104. *Intrinsic edge excitons in two-dimensional MoS2,* P. D'Amico, M. Gibertini, D. Prezzi, D. Varsano, A. Ferretti, N. Marzari, and E. Molinari, Physical Review B 101, 161410 (2020) DOI: 10.1103/PhysRevB.101.161410

105. *Magneto-optical response of chromium trihalide monolayers: chemical trends*, A. Molina-Sánchez, G. Catarina, D. Sangalli, and J. Fernández-Rossier, J. Mater. Chem. C, 8, 8856-8863 (2020) DOI: 10.1039/D0TC01322F

106. *Pump-driven normal-to-excitonic insulator transition: Josephson oscillations and signatures of BEC-BCS crossover in time-resolved ARPES*, E. Perfetto, D. Sangalli, A. Marini, and G. Stefanucci, Phys. Rev. Materials 3, 124601 (2019) DOI: 10.1103/PhysRevMaterials.3.124601

107. *Spin States Protected from Intrinsic Electron–Phonon Coupling Reaching 100 ns Lifetime at Room Temperature in MoSe2*, M. Ersfeld, F. Volmer, P. M. M. C. de Melo, R. de Winter, M. Heithoff, Z. Zanolli, C. Stampfer, M. J. Verstraete, and B. Beschoten, Nano Lett. 19, 4083-4090 (2019), DOI: 10.1021/acs.nanolett.9b01485

108. *Valley-engineering mobilities in 2D materials*, T. Sohier, M. Gibertini, D. Campi, G. Pizzi, and N. Marzari, Nano Lett. 19, 3723−3729 (2019), DOI: 10.1021/acs.nanolett.9b00865

General Article

109. *At SC21, Experts Ask: Can Fast HPC Be Green?*, Daniele Cesarini (CINECA), HPCWire article (30/11/2021) https://www.hpcwire.com/2021/11/30/at-sc21-experts-ask-can-fast-hpc-be-green/

ANNEX 3 - 3rd-party events

CATEGORY 1. Scientific conferences and workshops on HPC, targeting mostly the HPC community and HW stakeholders [HPC centres, technology partners] (as defined in D9.1 point 2.4)

#	Date	Event (title, place, participant, kind of contribution, link)
1	14/12/2020	**Nicola Marzari** (EPFL) *The great acceleration in the design and discovery of novel materials* Invited webinar at Materials Science Webinar, Università Tor Vergata (online) https://www.fisica.uniroma2.it/media/fprljcij/marzari.pdf
2	15/01/2021	**Giovanni Pizzi** (EPFL) *The technology stack to make simulations Accurate, Automatic and Available* Invited talk @ Workshop on Sector Day on Chemistry & Catalysis, online
3	29/01/2021	**Nicola Marzari** (EPFL) *The great acceleration in the design and discovery of novel materials* Webinar Colóquio da Nano - Universidade Federal do ABC (BR) - online https://eventos.ufabc.edu.br/evento/coloquio-da-nano-nicola-marzari/
4	03/03/2021	**Nicola Marzari** (EPFL) *The digital infrastructures for 21st-century science* Plenary talk @ 3RD EMMC INTERNATIONAL WORKSHOP EMMC 2021 – online https://emmc.eu/wp-content/uploads/2020/12/EMMC2021-P4-Marzari-Abstract.pdf
5	14/04/2021	**Andrea Ferretti** (Cnr) & **Ivan Carnimeo** (SISSA) *Materials Design Toward the Exascale: Porting Electronic Structure Community Codes to GPUs* Invited talk, GPU TECHNOLOGY CONFERENCE - GTC NVIDIA, online https://www.nvidia.com/en-us/gtc/call-for-submissions/
6	13/05/2021	**Nicola Marzari** (EPFL) *The great acceleration in the design and discovery of novel materials* ASHPC21 first Austrian-Slovenian HPC Meeting - online https://ashpc21.si/
7	16/06/2021	**Nicola Marzari** (EPFL) *Transport approaches* Talk @ MRS/ KAVLI Future of materials, online https://www.mrs.org/mrs-kavli-future-of-materials-virtual-workshop/
8	08/07/2021	**Andrea Ferretti** (Cnr) *Materials design towards the exascale: porting electronic structure community codes to GPU* PASC21 Geneva (CH) and online (hybrid) https://submissions.pasc-conference.org/pasc21_program/views/at_a_glance.html https://pasc21.pasc-conference.org/

9	15/09/2021	**Ivan Carnimeo** (SISSA) *New Developments of the Quantum ESPRESSO Code: A Combined* Talk @ OpenACC Summit 2021 - online https://www.youtube.com/watch?v=XcgkeS7V2_0 https://www.openacc.org/events/openacc-summit-2021
10	16-17/09/ 2021	**Elisa Molinari** (Cnr & Unimore) Ecosystem event: Second Biannual Meeting on Big-Map project - Copenhagen (DK)
11	28-29/09/ 2021	**Elisa Molinari** & **Nicola Spallanzani** (Cnr) *Materials design and supercomputing for Italian industry: The MaX CoE* Ecosystem event: Bi-Rex event https://bi-rex.it/en/events/
12	30/09/2021	**Giovanni Pizzi** (EPFL) *AiiDA, Materials Cloud, and common workflows for materials properties with 11+ different engines* Invited talk @ FAIR-DI workshop 2021, Louvain-la-Neuve (Belgium), online
13	06/10/2021	**Giovanni Pizzi** (EPFL) *Ontology-driven simulations with AiiDA and common workflows* Contributed talk @ Workshop on Ontologies for Materials-Databases Interoperability (OMDI2021), online https://liu.se/en/research/omdi2021
14	13/10/2021	**Giovanni Pizzi** (EPFL) *FAIR data and FAIR workflows with AiiDA: common workflows for materials properties with 11+ quantum engines* Invited talk @ EERAdata joint workshop “FAIRification put into practice”, online https://www.eeradata.eu/event/3028:eeradata-workshop-no-3-fairification-put-into-practice.html
15	1-3/11/ 2021	**Nicola Marzari** (EPFL) *Exascale challenges in low dimensional materials* Joint Nomad - E-cam workshop “Modeling Materials at realistic space and time scales via optimal exploitation of exascale computers and AI” https://nomad-coe.eu/events/nomad-e-cam-workshop
16	11/11/2021	**Flaviano dos Santos** & **Marnik Berck** (EPFL) *Generating a fair crystal-structure database with the AiiDa informatics platform* Contributed talk @ Intnl Workshop on Advanced material-to-device solutions for synaptic electrons (H2020 Intersect) - Barcelona (ES)
17	15/11/2021	**Giovanni Pizzi** (EPFL) *High-throughput and provenance with AiiDA and common workflows* Invited talk @ High-throughput workflows for materials science with the atomic simulation environment (ASE) and fireworks, Lyngby, Denmark
18	17/11/2021	**Daniele Cesarini** (CINECA)

		Can Fast Be Green? Opportunities and Challenges for Europe When Making HPC Sustainable -Virtual Birds of a Feather at Supercomputing (SC) 2021 https://sc21.supercomputing.org/presentation/?id=bof104&sess=sess353
19	18/11/2021	**Giovanni Pizzi** (EPFL) *Data-enabled modelling with AiiDA: towards autonomous laboratories* Invited talk @ Data enabled atomistic modelling, Abingdon, United Kingdom https://www.scd.stfc.ac.uk/Pages/CoSeC_CoSeC_CECAM_wkshp.aspx
20	02/03/2022	**Elisa Molinari, Nicola Spallanzani, Andrea Ferretti** (CNR) Intel oneAPI Workshop - online
21	15/03/2022	**Nakib H Protik** (ICN2) *elphbolt: An ab initio solver for the coupled and decoupled electron and phonon Boltzmann transport equations (GA48.00003)* Contributed talk @ APS March Meeting 2022 - Chicago, IL (US)
22	08/04/2022	**Laura Bellentani** (CINECA) *Car-Parrinello Molecular Dynamics: a use case for ADMIRE* Webinar online for the ADMIRE project https://www.admire-eurohpc.eu/Dissemination/
23	19/05/2022	**Daniele Cesarini** (CINECA) *Microarchitecture performance assessment and energy monitoring of MaX codes through Linux Perf and power management API interfaces* Invited talk at HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING (HPCSE) https://hpcse.it4i.cz/HPCSE22/
24	20/05/2022	**Marnik Berckx** (EPFL) *AiiDA - Automated Interactive Infrastructure and Database for Computational Science* Talk @ AiiDA tutorial, Antwerp (BE) https://www.uantwerpen.be/en/projects/antwerp-young-minds/activitites/
25	29/05/2022 - 02/06/2022	**Workshop on Software Co-Design Actions in European Flagship HPC Codes** @ ISC2022, Amburgo (DE) https://www.isc-hpc.com/ - **Fabrizio Magugliani** (E4), booth - **Daniele Cesarini** (E4), *Performance Assessment and Energy Efficiency of MaX Codes* (Invited talk) - **Conrad Hillairet** (ARM), Organization
26	22/06/2022	**Marnik Berckx** (EPFL) *AiiDA and Materials Cloud* Invited Talk @ 15th International Ceramics Congress, Perugia (IT) http://2022.cimtec-congress.org/

27	29/06/2022	**Nicola Marzari** (EPFL) *There is plenty of room at the top: novel 2-dimensional materials from the computational exfoliation of all known compounds.* Invited talk for Prace HPC Excellence Award @PASC 2022, Basel (CH) https://www.youtube.com/watch?v=01G8sbz5u-8&list=PLeU4yWBiw8ja4CGHTSqQua056hVLmREhw&index=11 https://pasc22.pasc-conference.org/program/keynote-presentations/index.html
28	23/08/2022	**Francesco Ramirez** (EPFL) *AiiDA and the data provenance model* Talk @ Love Data Week 2021 at EPFL, Lausanne (CH)https://memento.epfl.ch/event/love-data-week-2021-at-epfl-2/
29	24/08/2022	**Anton Kozhevnikov** (ETHZ/CSCS) *Portfolio of CSCS libraries for electronic structure applications* Contributed talk @ Psi-K 2022 - Lausanne (CH) https://www.psik2022.net/
30	12/09/2022	**NVIDIA roundtable**, CINECA, Casalecchio del Reno (BO) - **Laura Bellentani** & **Sergio Orlandini** (CINECA); **Andrea Ferretti** & **Nicola Spallanzani** (Cnr) - **Ivan Carnimeo** (SISSA), *Quantum ESPRESSO* (Talk) - **Andrea Ferretti** (CNR), *Materials design towards the exascale: porting electronic structure community codes to GPU* (Invited presentation)
31	3-5/10/ 2022	**Andrea Ferretti** (CNR) International Workshop on Co-Design for HPC in Computational Materials and Molecular Science - Lausanne (CH). 1113 Workshop organized jointly with NOMAD, TREX and Bioexcel https://www.cecam.org/workshop-details/
32	13-18/11/ 2022	**CINECA Booth** with MaX materials @ SC22 Dallas (USA) http://sc22.supercomputing.org/

CATEGORY 2. Scientific conferences and workshops in materials science and engineering, physics and chemistry, targeting mostly end-users of materials simulations in industry and academia [codes & ecosystem developers].

#	Date	Event (title, place, participant, kind of contribution, link)
33	23-25/02/ 2021	**Claudia Pereira Cardoso** (CNR) *POSTER: Electronic and magnetic properties of well defined Gr/Co/Ir(111) and Gr/Fe/Ir(111) heterostructures* TOTAL ENERGY - 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods – online http://indico.ictp.it/event/9510/overview; http://indico.ictp.it/event/9510/material/10/0.pdf
34	2-3/03/2021	**Andrea Ferretti** & **Daniele Varsano** (Cnr) *A journey through electronic structure and materials modelling at the exascale*

		CoEs' POSTER exhibition: 3RD EMMC INTERNATIONAL WORKSHOP EMMC 2021, online https://emmc.eu/emmc-2021/program/virtual_contribution/feretti-versano/
35	15-19/03/ 2021	**APS March Meeting 2021 -** online. - **Alberto Guandalini** (Cnr), *B57.00003: Efficient GW calculations in two dimensional through the interpolation of the screened potential* (Contributed talk) - **Dario Leon Valido** (Cnr), *C22.00002: Frequency dependence of W made simple using a multi-pole approximation* (Contributed talk) - **Claudia Pereira Cardoso** (Cnr), *B57.00003: Efficient GW calculations in two dimensional through the interpolation of the screened potential* (Contributed talk) - **Miki Bonacci** (Cnr), *R57.00007: Excitonic dispersion in monolayer C3N* (Contributed talk) - **Giacomo Sesti** (Cnr), *R41.00002: Excitonic vs Mott insulator in carbon nanotubes: A proposed experimental test* (Contributed talk) - **Massimo Rontani** (Cnr), *V57.00006: Evidence of ideal excitonic insulator in bulk MoS2 under pressure* (Contributed talk) - **Simone Vacondio** (Cnr), *R22.00007: Higher order many-body perturbation theory applied to atomic systems* (Contributed talk) - **Paolo Pegolo** (SISSA), *M20.00011: Oxidation states, Thouless' pumps, and nontrivial transport in nonstoichiometric electrolytes* (Contributed talk) - **Pablo Ordejón** (ICN2), *Addressing electrified metal-electrolyte interfaces with Non-Equilibrium Green's Functions* (Invited talk) - **Davide Tisi** (SISSA), *Heat transport in water from Deep Neural Network potentials* (Contributed talk) - **Stefano Baroni** (SISSA), *M20.00001: Gauge invariance of heat and charge transport coefficients* (Invited talk) - **Miriam Winkelmann** (Jülich), *M22.00009: Kerker mixing scheme for self-consistent muffin-tin based all-electron electronic structure calculations* (Contributed talk) - **Marnik Berck** (EPFL), *M41.00004: Generating a FAIR crystal-structure database with the AiiDA informatics infrastructure* (Contributed talk) - **Giovanni Pizzi** (EPFL), *Shear and breathing modes of all layered materials* (Contributed talk)
36	14-18/06/ 2021	**Paolo Giannozzi** (CNR) *Lecture: Density-Functional Perturbation Theory* Virtual 2021 School on Electron-Phonon Physics from first principles - Austin, USA (online) http://docs.epw-code.org/doc/School2021.html
37	17-18/06/ 2021	**Daniele Varsano** (CNR) *Evidence of exciton instability in T' −MoS2 and bulk MoS2 under pressure* Invited talk @ 2Day A two-day meeting on the progress of two-dimensional materials; Rome, La Sapienza https://www.chem.uniroma1.it/en/news/2day-a-two-day-meeting-on-the-progress-of-two-dimensional-materials
38	22/06/2021	**Daniele Varsano** (CNR) *Evidence of ideal excitonic insulator in MoS2 under pressure*

		Invited talk @ Cecam workshop: Excitonic and competing orders in low-dimensional materials; online https://www.cecam.org/workshop-details/21
39	13/07/2021	**Pablo Ordejón** (ICN2) *Addressing electrified metal-electrolyte interfaces with Non-Equilibrium Green's Functions* Invited talk @ Workshop on "Water: Grand Challenges for Molecular Science and Engineering", Telluride Science Research Center, Telluride (US) https://www.telluridescience.org/meetings/workshop-details?wid=953
40	31/08/2021	**Elisa Molinari** (Cnr & Unimore) *The exciton that you might not expect* Keynote lecture @ Chem2Dmat2021 - online http://phantomsfoundation.com/CHEM2DMATCONF/2021/Abstracts/Chem2Dmatconf2021_Molinari.pdf; http://www.chem2dmatconf.org/2021/
41	24/09/2021	**Andrea Ferretti** (Cnr) *Coherent electron transport through molecular nanojunctions* Invited lecture @ MSSC21 - London (UK) https://www.imperial.ac.uk/mssc/mssc2021/
42	06/10/2021	**Pablo Ordejón** (ICN2) *Towards first-principles electrochemistry: Addressing electrified metal-electrolyte interfaces with DFT-NEGF* Keynote talk @ TNT2021 Conference, Tirana (Albania) https://tntconf.org/2021/programme.php?d=06
43	21-22/10/2021	**Cecam workshop: Recent developments in quantum Monte Carlo**. Rome, Enrico Fermi Research Centre - **Stefano Baroni** (SISSA), *Stochastic perturbation theory* (Invited talk) - **Daniele Varsano** (Cnr), *Evidence of ideal excitonic insulator in MoS2 under pressure* (Invited talk) https://www.cecam.org/workshop-details/1050
44	10-13/01/2022	**Thierry Deutsch** (CEA) *New formalism for the exact calculation of total energies and associated electronic state of many-body interactions with complexity n^6* GdR NBODY General Meeting - Toulouse, France https://lcpq.github.io/gdr_nbody_2021/presentations/deutsch.pdf https://lcpq.github.io/gdr_nbody_2021/
45	24/02/2022	**Daniele Varsano** (Cnr) *Hunting excitonic instabilities in low dimensional systems* Colloquium @ Colloquium Series in Theoretical and Computational Physics (CSTCP) - Physics Department of the University of Trieste, Italy https://www.youtube.com/watch?v=Kd9yHfA7WPc
46	25/02/2022	**Davide Sangalli** (Cnr)

		Ab initio approach to exciton dynamics Invited seminar @ ETSF Seminar -online https://psi-k.net/events/etsf-online-seminar-by-davide-sangalli-friday-feb/
47	11/03/2021	**Giovanni Pizzi** (EPFL) *The powerful synergies of high-throughput simulations and physical intuition* Invited talk @ TechTalk DTU - online
48	14-16/03/ 2022	**APS March Meeting 2022** - Chicago, IL (US). Invited talks: - **Andrea Marini** (Cnr), *N46.00001: Photo-induced phase-transitions and coherent phenomena in realistic materials: an ab-initio Many-Body approach* - **Nicola Marzari** (EPFL), *Charting the electronic structure of inorganic materials* Contributed talks: - **Christian-Roman Gerhorst** (Jülich), *W46.00008: Calculating Phonons within the FLAPW Method using Density Functional Perturbation Theory (DFPT)* - **Alberto Guandalini** (Cnr), *G66.00005: Efficient GW calculations in two dimensional through the interpolation of the screened potential* - **Dario A Leon Valido** (Cnr), *A multipole approach for dielectric screening in metallic systems* - **Chunhua Li** (ICN2), *G48.00007: Coupled electron-phonon transport from first principles*
49	15-18/05/ 2022	**Ernane de Freitas Martins** (RMIT-ICN2) *A multiscale QM/MM + NEGF approach to address electrified metallic-water interfaces* Contributed talk @ Electrified solid/water interfaces - theory meets experiments workshop - Tegernsee (Germany) https://www.mpie.de/eswi22
50	13-19/06/ 2022	**Paolo Giannozzi** (CNR) *Density-Functional Perturbation Theory* Lecture @ 2022 School on Electron-Phonon Physics from first principles Austin, USA https://epw2022.oden.utexas.edu/https://epw2022.oden.utexas.edu/
51	15-17/06/ 2022	**Thierry Deutsch** (CEA) *N-representable parametrization of the 2RDMs based on a new compact formalism Grenoble Conference* International Conference on Reduced Density Matrix Theory for Quantum Many-Fermion Systems (RDM2022) - Donostia-San Sebastian, Spain
52	20-23/06/ 2022	**Ernane de Freitas Martins** (RMIT-ICN2) *Electrified metallic-water interfaces from a QM/MM + NEGF approach* Contributed talk @ Present and future of hybrid quantum chemical and molecular mechanical simulations workshop - Lecco (Italy) https://www.cecam.org/workshop-details/1152
53	03/07/2022	**Deborah Prezzi** (CNR)

		Illuminating low-D Materials: Insights into Electronic and Optical Spectroscopies from First Principles Simulations Invited lecture @ Xenes-4 & Epioptics-16, Intnl School of Solid State Physics - Erice (IT) https://www.ism.cnr.it/it/news/archivio-news/item/92-epioptics-16.html
54	25/07/2022	**Pablo Ordejón** (ICN2) *Towards first-principles simulations of electrochemical processes at the nanoscale* Invited talk @ Mole Conference 2022 - San Sebastian (Spain) http://moleconference2022.dipc.org/program
55	22-25/08/ 2022	**Psi-K 2022** - Lausanne (CH) https://www.psik2022.net/ Invited talks: - **Stefano Baroni** (SISSA), *Topology, oxidation states, and charge transport in ionic conductors* - **Stefan Blügel** (Jülich), *Magnetic Skyrmions – Scientific fascination through ab initio theory* - **Thierry Deutsch** (CEA), *Exact solution of the many-body problem with a $O(n^6)$ complexity* - **Andrea Ferretti** (Cnr), *Dynamical potentials to get both total energy and spectral properties* - **Daniele Varsano** (Cnr), *Evidence of ideal excitonic insulator in MoS2 under pressure* Contributed talks: - **Pino D'Amico** (Cnr), *Intrinsic edge excitons in two-dimensional MoS2* - **Roberta Farris** (ICN2), *Lattice thermal conductivity of Transition Metal Dichalcogenides: from monolayer to bulk* - **Christoph Friedrich** (Jülich), *Electron-plasmon and electron-magnon scattering in ferromagnets from first principles by combining GW and GT self-energies* - **Federico N. Pedron** (ICN2), *On-the-fly basis set contraction in SIESTA: performance and usability* - **Giovanni Pizzi** (EPFL), *An all-chemistries comprehensive verification of all-electron and pseudopotential DFT codes via universal common workflows* - **Miguel Pruneda** (ICN2), *Dynamic control of octahedral rotation of perovskites by defect engineering* - **Davide Sangalli** (Cnr), *Excitons with the yambo code: from the Bethe-Salpeter equation to nonequilibrium excitons and exciton-phonon coupling* - **Nils Wittemeier** (ICN2), *Quantum transport with Spin-Orbit Coupling* Poster - **Francesco Ramirez** (EPFL), *High-throughput identification of novel electrides via automated AiiDA workflows* - **Christian-Roman Gerhorst** (Jülich), *Calculating Phonons within the FLAPW Method using Density Functional Perturbation Theory (DFPT)* - **Alberto Guandalini** (Cnr), *Efficient GW calculations in two dimensional materials through a stochastic integration of the screened potential* - **Gregor Michalicek** (Jülich), *Automatized determination of high-precision setup parameters for all-electron FLAPW calculations with the FLEUR code*

		- ***Daniel WORTMANN*** (Jülich), *Path to exascale computing with the all-electron DFT code FLEUR*
56	26/08/2022	**Pablo Ordejón** (ICN2) *Democratization of DFT: A European Perspective* APS Meyer Hall Celebration - Birthplace of Density Functional Theory, UC San Diego (USA) https://ucsdnews.ucsd.edu/pressrelease/mayer-hall-recognized-for-historical-contributions-to-physics
57	14/09/2022	**Alberto García** (CSIC) *Participation in roundtable discussion* FAIRmat workshop on data quality in DFT codes, Co-organized by NOMAD https://www.fairdi.eu/events/fairmat-workshop-on-data-quality-in-dft-codes
58	23/09/2022	**Andrea Ferretti** (Cnr) *Coherent electron transport through molecular nanojunctions* Invited lecture @ MSSC22 - London (UK) https://www.imperial.ac.uk/mssc/mssc2022/

CATEGORY 3. Events aimed at engaging with the policy ecosystem.

#	Date	Event (title, place, participant, kind of contribution, link)
59	12/03/2021	**Focus CoE CoEs Co-Design Workshop** (online) - Session 1 Different levels of co-design, where do CoEs come in?, **Fabio Affinito** (Cineca), panelist - Session 2 Co-Design for new usage, **Leopold Talirz** (EPFL), panelist
60	23/03/2021	**Elisa Molinari** (Cnr & Unimore) & **Joost VandeVondele** (CSCS ETHZ) *Support in EuroHPC - Status and Future: Centres of Excellence in Context* Panelists in "CoEs on the road to Exascale Session" organized by FocusCoE; EuroHPC Summit Week 2021 – online https://events.prace-ri.eu/event/1018/timetable/#20210323.detailed
61	24/03/2021	**MaX CoE Workshop**: Computational Materials Design at the Exascale: porting community codes, challenges and success cases. EuroHPC Summit Week 2021 - online. Contributes: - **Andrea Ferretti** (Cnr): Welcome - **Nicola Marzari** (EPFL): Materials design at the intersection of high-throughput and high-performance-computing - **Stefano Baroni** (SISSA): Challenges and success towards the exascale: the perspective of Quantum ESPRESSO, a large community code - **Joost VandeVondele** (ETHZ): Software engineering towards exascale: domain specific libraries, communication optimality, and machine learning - **Daniele Varsano** (Cnr): Accelerating GW and many-body perturbation theory using GPUs: yambo hunting for excitonic insulators

		- **Uliana Alekseeva** (Jülich): Parallelization and optimization of the FLEUR code: new possibilities for all-electron Density Functional Theory - **Pablo Ordejón** (ICN2): HPC-enabled very large scale quantum simulations in materials with SIESTA https://events.prace-ri.eu/event/1018/timetable/#20210324.detailed
62	02/06/2021	**Elisa Molinari** (Cnr & Unimore) Invited panelist on HPC during the Digital Day "Leading the Digital Decade DIGITAL EUROPE PROGRAMME" - online https://digital-strategy.ec.europa.eu/en/policies/leading-digital-decade https://www.youtube.com/watch?v=hFCMkGdhvlQ
63	26/10/2021	**Elisa Molinari** (Cnr & Unimore) *HPC and Big Data as key enablers of the Clean Energy Transition* (panel with other CoEs EoCoE, MaX, HiDALGO, HVL, and FocusCoE) Energy Talk 3795 - EUSEW21 EU Sustainable Energy Week - (online)
64	9-10/11/ 2021	**Elisa Molinari** (Cnr & Unimore) Participant in EU-Japan workshop on HPC-based material sciences (online) [policy making event]
65	22-24/03/ 2022	**EuroHPC Summit Week 2022** - Paris (FR) - **Elisa Molinari** (Cnr & Unimore) & **Fabrizio Magugliani** (E4), *Discussion/Q&A* with F. Magugliani (*ET4HPC*) and E. Molinari (former RIAG Member) - **Ivan Carnimeo** (SISSA), *Quantum ESPRESSO on GPU: accelerating a complex code combining performance with portability* (Talk) - **Marnik Berckx** (EPFL), *Generating a FAIR crystal-structure database with the AiiDA informatics infrastructure* (Talk) - **Daniel Wortmann** (Jülich), *Large scale electronic structure simulations of complex magnetic objects* (Talk) https://events.prace-ri.eu/event/1214/page/142-pracedays22-call-for-contributions

CATEGORY 4. Third-party workshops and conferences that aim to train research and academia students.

#	Date	Event (title, place, participant, kind of contribution, link)
66	15-16/03/20 21	**Nicola Marzari** & **Giovanni Pizzi** (EPFL) *The AiiDA & Materials Cloud informatics platform for complex workflows* Simulation Workflows in Materials Modeling – SWiMM 2021 workshop – online
67	11/10/2021	**Alberto García** (CSIC) *Library integration in Siesta: challenges and opportunities* Invited talk @ ESL Extended Software Development Workshop: Improving bundle libraries https://www.cecam.org/workshop-details/23

68	12/10/2021	**Giovanni Pizzi** (EPFL) *AiiDA, Materials Cloud, and common workflows for materials properties with 11+ different engines* Invited talk @ Extended Software Development Workshop: Improving bundle libraries, Lausanne, Switzerland https://www.cecam.org/workshop-details/23
69	13-19/06/2022	**Paolo Giannozzi** (CNR) *Density-Functional Perturbation Theory and Additional contributions to the code: Debug and code alignment with QE* Invited talk at Virtual 2022 School on Electron-Phonon Physics from first principles - Austin, USA 13-19/06/2022 https://epw2022.oden.utexas.edu/https://epw2022.oden.utexas.edu/
70	19/07/2022	**Daniel Wortmann** (Jülich) *All-electron DFT heading to exascale: new possibilities for virtual materials design* Invited talk @ CECAM Flagship Workshop Virtual Materials Design - Karlsruhe Institute of Technology, Germany https://www.cecam.org/workshop-details/1143
71	20-21/07/2021	**Nicola Marzari** (EPFL) *Digital infrastructures for materials discovery: the convergence of databases, simulations, and accelerators* Talk @ CECAM-Workshop Virtual Materials Design 2021 - Session Materials acceleration – online https://www.cecam.org/workshop-details/1093
72	20/11/2021	**Anton Kozhevnikov** (ETHZ/CSCS) *SIRIUS: a GPU accelerated plane-wave DFT library* Contributed talk @ "Extended Software Development Workshop: Improving bundle libraries" - CECAM-HQ-EPFL, Lausanne, Switzerland https://www.cecam.org/workshop-details/23
73	13/12/2021	**Anton Kozhevnikov** (ETHZ/CSCS) *Libraries for electronic structure community* Contributed talk at the "MolSSI Workshop on HPC in Computational Chemistry and Materials Science" - Berkeley, CA, USA https://wordpress.cels.anl.gov/molssi-hpc/
74	09-13/05/2022	**Stefano De Gironcoli** (SISSA) Organizer: International Workshop "Psi-k: Young Researcher's Workshop on Machine Learning for Materials" - Trieste (Italy), SISSA Miramare Campus https://ml4m.xyz/
75	14/09/2022	**Gregor Michalicek** (Jülich) *Challenges in comparing LAPW calculations and estimating their precision* Talk @ FAIRmat workshop on data quality in DFT codes - online

CATEGORY 5. Third-party events on outreach.

#	Date	Event (title, place, participant, kind of contribution, link)

76	31/05/2021	**Nicola Marzari** (EPFL) *Materials discovery at the intersection between high-performance and high-throughput AI and ML in Materials Design and Discovery* - online
77	21/06/2021	**Nicola Marzari** (EPFL) *The Great Acceleration in Materials Discovery* Webinar speaker @ nexFrontier series - Novel Materials Discovery, The Marvel Of Computational Science - online https://swissnex.org/china/event/nexfrontier-novel-materials-discovery-the-marvel-of-computational-science/
78	23/11/2021	**Nicola Marzari** EPFL *The Great Acceleration in the Design and Discovery of Novel Materials* Webinar online / The Cyprus Institute https://www.cyi.ac.cy/index.php/component/k2/webinar-the-great-acceleration-in-the-design-and-discovery-of-novel-materials.html
79	21-22/01/ 2022	**Elisa Molinari** (Cnr & Unimore) Organizer & Chair of Convegno Annuale Associazione Donne e Scienza, Modena (IT) https://donnescienza2022.nano.cnr.it/
80	23-24/09/ 2022	Trieste Next: Festival della ricerca scientifica - Trieste (Italy) - **Elisa Molinari** (Cnr & Unimore), **Nicola Marzari** (EPFL), **Stefano Baroni** (SISSA), *Quantum Alchemy: How Computers Help Create New Materials* (Panel discussion) https://www.triestenext.it/tc-events/quantum-alchemy-how-computers-help-create-new-materials - **Nicola Marzari** (EPFL), *A universe within a chip: crossing the frontiers of knowledge with a super-computer,* Panel discussion https://www.triestenext.it/tc-events/a-universe-within-a-chip-crossing-the-frontiers-of-knowledge
81	30/09/2022	**Marco Gibertini**, **Giacomo Sesti**, **Claudia Cardoso** (Cnr), *Designing the future of electronics*. CNR, European Research Night 2021 & 2022, Modena (IT)

CATEGORY 6. upcoming events

#	Date	Event (title, place, participant, kind of contribution, link)
82	10-17/10/ 2022	**Pietro Delugas** (SISSA) *Quantum ESPRESSO core libraries and their pivotal role for multiplatform support* CECAM Workshop: Electronic Structure Software Development: Best Practices and Tools - Lausanne (CH) https://www.cecam.org/workshop-details/1121
83	3-5/10/2022	**Alberto García** (CSIC) *A modular SIESTA as a vehicle for co-design*

		International Workshop on Co-Design for HPC in Computational Materials and Molecular Science Lausanne (CH) Joint Workshop with NOMAD, TREX and Bioexcel https://www.cecam.org/workshop-details/1113
84	10-11/10/ 2022	**Alberto García** (CSIC) *Outlook and wish-list for "best practices" from the experience in the SIESTA ecosystem* Electronic Structure Software Development: Best Practices and Tools Lausanne (CH) ESL Workshop https://www.cecam.org/workshop-details/1121