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D4.9

Second report on dissemination and communication activity

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Document information

Project acronym:	INTERSECT
Project full title:	Interoperable Material-to-Device simulation box for disruptive electronics
Research Action Project type:	Accelerating the uptake of materials modelling software (IA)
EC Grant agreement no.:	814487
Project starting / end date:	1st January 2019 (M1) / 30th April 2022 (M40)
Website:	www.intersect-project.eu
Final version:	29/04/2022
Deliverable No.:	D4.9
Responsible participant:	CNR (participant number 1)
Due date of deliverable:	30/04/2022
Actual submission date:	29/04/2022
Dissemination level:	PU - Public

Authors:	Luisa Neri, Maria Bartolacelli, and Arrigo Calzolari
To be cited as:	L. Neri, M. Bartolacelli, and A. Calzolari (2022): Second report on dissemination and communication activity. Deliverable D4.9 of the H2020 project INTERSECT (final version as of 29/04/2022). EC grant agreement no: 814487, CNR, Modena, Italy

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Versioning and Contribution History

Version	Date	Modified by	Modification reason
v.01	20/04/2022	Maria Bartolacelli and Luisa Neri	First version
v.02	27/04/2022	Matthias Büschelberger	Second revision
v.03	28/04/2022	Arrigo Calzolari	Final version

Content

Executive Summary

The deliverable D4.9 "Second report on dissemination and communication activities", deals with the communication and dissemination activities implemented to promote, diffuse, and share the INTERSECT project and its results from M20 to M40. It delivers the results of activities performed within WP4 "Exploitation, dissemination and communication", in particular in Task 4.2 "Dissemination activities", Task 4.3 "Communication activities". The WP4 is led by CNR Nano, with a proactive participation of all partners.

A special attention has been paid in this period to plan and actuate actions directed to an industrial audience, in order to make them aware of our Interoperable Material-To-Device Simulation Box (IM2D). To this end we were awarded a 3-month extension, aimed at implementing activities oriented to dissemination, to an increased industrial uptake and sustainability, to training, and to widening the community's involvement.

Thanks to this extension, we were able to complete and finalize the IM2D toolbox and foster the dissemination activity toward the semiconductor community. In this frame, along with a thick activity of communication and dissemination via talks and publications, we organized three well-participated tailored events: a hybrid international workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics (Nov. 2021), a hands-on webinar on Combining semantic web technologies with automated workflows within the IM2D simulation tool box (Mar. 2022), and a webinar on IM2D to present the simulation box for disruptive electronics (Apr. 2022).

1.   Introduction

INTERSECT is a multidisciplinary project for the realization of the Interoperable Material-To-Device Simulation Box (IM2D) that is conceived as an interoperable, robust, and friendly software solution for advanced materials modelling from an electronic device-oriented industrial perspective. In particular, IM2D aims at enabling the simulation-aided design and optimization of devices for disrupting electronics (e.g., storage class memories, selectors, etc). The project also aims at the development and the implementation of new features in materials and device modelling codes, automatic workflows, interoperability modules, development of materials-oriented ontology, design, and optimization of complex materials and electronic devices, materials database population, integration with EU cloud infrastructures (e.g., European Materials Marketplace). Thus, all the advances in software

production, electronics and technology, scientific knowledge, and interoperability uptakes obtained during the project are valuable results to communicate and disseminate. The variety of the outcomes demands also for a diversification of the target audience. Potential interested stakeholders include electronics engineers, physicists, materials scientists, academic and public institutions, software vendors, semiconductor industries, and general audience. Each stakeholder requires a specific communication level and specific communication tools.

In the early months of the projects, we focussed on setting objectives, defining means, and selecting target audiences, while in this second part we were able to put in place a great deal of activities aimed at the communication and dissemination of our results that in the meantime had come out.
On the one hand, we planned a day-to-day communication via social media and the website (see Section 4). On the other hand, along with dissemination of scientific results (e.g., thermal transport through amorphous chalcogenides for selectors), we put a lot of effort in promoting, especially for industrial uptake, our IM2D box (see Section 3).

Collaborations with similar projects and the EU ecosystems as well as a complete list of publications and talks complete this report.

Important note: Because of the worldwide restrictions due to COVID-19, public activities that require in person attendance (such as participation/organization to/of workshops, conferences, training courses, seminars) have been almost completely substituted by online formats. Though we adapted to this format quickly, and did our best not to hamper our activities, we deem that this situation has lowered the possible impact of dissemination events.

2.   Dissemination and Communication Report

The Intersect project has invested in communication and dissemination activities since its proposal, as it is reckoned very important to share the results of a public-funded research project and because it is very useful for the growth of the project itself, the building of an interested community. Many tools were identified, and relevant audiences and KPIs set for the activity to perform.

In the project coordinator (PC)'s node CNR a communication officer, dr. Mara Di Berardo, was hired for this purpose and was active from M18 (due to delays in hiring policies) to the end of M37. Whereas many activities were started in the earlier months, the dedication of a professional boosted the content preparation and management, as well as the networking within the consortium.

In the following, the Dissemination and communication plan (as adapted in D4.4, Tables 3 and 4) has been completed to report all results at M40.

Target	Scientific community
Channels	Participation in conferences; Publications in peer reviewed journals.
Indicators	10 or more conference contributions; 6 or more publications in journals or conferences.
Outputs	36 Conference contributions /invited or contributed talk + 5 posters) in 21 events. 14 papers already published https://intersect-project.eu/publications/ + 4 submitted or manuscript in preparation.
Target	Scientific and industrial community
Channels	Conferences; Webinars, showcases or workshops; training courses.
Indicators	Organisation of at least two webinars or showcases, and one training course.
Outputs	2 training courses (RP1): Tutorial on writing reproducible workflows for computational materials science (May 21-24, 2019 - online), AiiDA Virtual Tutorial (July 7-10, 2020 - online), 2 webinars (RP2): TechCafé (March 29, 2022 - online), IM2D Webinar (April 27, 2022 - online)

Table I. Dissemination report (adapted from Table 2, D4.4).

Target	Industrial community, scientific community, public at large
Channels	Public deliverables and articles, brochures, press releases, newsletter. Final meeting to exchange knowledge received during the project, to reveal optimization potential for further development and thus be the initial event for subsequent cooperation projects.
Indicators	1 brochure, 1 press release, 1 newsletter every 12 months, articles posted on the project website. 1 final meeting (open to public at large). Social network posts and weekly management. Website weekly management.
Outputs	1 flyer (release date 05/08/2021) 2 press releases: https://icn2.cat/en/news/4363-an-intersect-meeting-to-boost-disruptive-electronicshttps://icn2.cat/en/news/4781-international-workshop-on-advanced-materials-to-device-solutions-for-synaptic-electronics-1 2 newsletters: issue n. 1 (12/03/2021) and issue n. 2 (17/03/2022). 101 news posted on the project website (75 in RP2). 1 International Workshop on Advanced Materials-to-device Solution for synaptic electronics - held in Barcelona (November 10-12, 2021). 629 posts on Twitter (347 in RP2). 115 posts on LinkedIn (last year). 280 posts on Instagram (273 in RP2).
Target	**Public at large**
Channels	Newsletters dedicated to general public; speeches during open days organised by the partners.
Indicators	All project public deliverables published on the website. At least one newsletter about the project to be published in local language in all participating regions. Participation to open days initiatives and other public events.
Outputs	All project public deliverables have been published on the website. M40 deliverables will be added. Public activities have been prevented by the pandemic.

Table II. Communication report (adapted from Table 2, D4.4).

The outputs from the tables above show that the activity has been fully performed (but for public events, mainly due to the pandemic) and the efforts of dissemination and communication have helped create a community consciousness of INTERSECT results. Most scientific results and technical achievements have been delivered on time, but the consortium deemed it useful to ask for an extension (AMD-814487-11, date 8/11/2021) in order to have more time to present to the industrial and research public its main result, the IM2D box, which came at full development at the foreseen end of the project. Its exploitation will continue after the end of the project.

3.   IM2D Events

One of the main objectives of INTERSECT has been, since the beginning, the development of the IM2D tool, an integrated, standardized, interoperable software platform conceived for the direct and easy exploitation by industrial users to accelerate the development of emerging electronic devices such as FeFET, memristors (PCM, RRAM), and selectors. It is based on a multi-physics (DFT, MonteCarlo, electrodynamics) and multiscale approach with focus on novel, complex, "real life" materials in the specific device configuration. IM2D conjugates the advantages of material and device-driven software, connecting the properties of materials at the atomistic level to the electrical behaviour of devices, with the aim to reduce the gap between materials and device realms and sustain the simulation-aided R&D processes of semiconductor industries and SMEs.

This last feature of sustaining the simulation-aided R&D processes of industries and SMEs has been at the centre of many communication activities of ours. The project and the development of IM2D at the beginning, and its realisation then have led to many dissemination activities for its uptake by potential users.

Dedicated pages on the website, with images, videos, and printables have been available for a while, but in the last months our main concern has been the planning and organization of three IM2D-related main events.

The three events, detailed below, are:

1) The "International Workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics", Barcelona (ES) and online, November 10-12, 2021.
2) The TechCafé "Combining semantic web technologies with automated workflows within the IM2D simulation toolbox", online, March 29, 2022.

3) The "IM2D webinar: Presenting the simulation box for disruptive electronics",
online, April 27, 2022.

Even though all three events were open to all interested attendees from academy, R&D
labs, and industry, we intentionally diversified the target and the focus of each meeting in
order to best encounter the different audience interests. 1) The meeting in Barcelona was
focused on the identification of the most urgent scientific problems which attain the
development of novel electronic solutions. Large space was dedicated to the presentation
and the discussion of the most recent experimental findings in the field of synaptic
electronics. This allowed us to present our results, but also to gain a direct insight on the
present and future interest of industrial producers. 2) The TechCafé was focused on the
implemented interoperability features (e.g., automated workflows, semantic
interoperability) of the IM2D box. The subject was more technical and mostly dedicated to
people expert/interested in automation processes, including users in the field of
industrial/commercial modelling (e.g., CAD-aid solutions). 3) The webinar was focused on
the presentation of the IM2D code to interested early users, with specific attention to
description of the aspects (and the corresponding computational features) that can be of
major interest to industrial users (also in term of costs, data protection, licences, HPC
resources), so to combine the solution of state-of-the-art technological problems, with a
user-friendly access to the code, also to not-experts in advanced simulations.

3.1 The "International Workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics" - Barcelona (ES) and online, November 10-12, 2021

Figure 1. The INTERSECT workshop banner.

WHAT. The **"International Workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics"** was organized by the INTERSECT partners with the aim of connecting academic research, R&D labs, and industry on the theme of synaptic electronics and neuromorphic computing, with a specific focus on the role of materials on the efficiency and design of next-generation devices.

It took place on November 10-12, 2021, at Casa de la Convalecencia, UAB, in Barcelona (ES) and online. The pandemic situation loosened its grip at that time, and we were able to hold the meeting in person. All the INTERSECT PIs served in the scientific committee of the workshop, while CNR and ICN2 took the role of organizers. No fee was required to participants.

HOW. The International workshop was organized in four half-day sessions, with 20 talks from invited speakers, project partners, or contributors. The topics of the sessions covered all areas of interest and keywords of the project, covering fields of interests from science to computation to future perspectives, and were:

- Session 1. Ferroelectrics device and materials (10/11/2012).
- Session 2. Interoperability, Ontology and Workflow in Materials Modelling (11/11/2021).
- Session 3. Alternative solutions for neuromorphing computers (11/11/2021).
- Session 4. PCM device and materials (12/11/2021).

Figure 2. F. Dos Santos (EPFL), M. Büschelberger (Fraunhofer IWM), M. Bertocchi (AMAT) presented the IM2D demonstrator at the INTERSECT workshop.

Eight talks were given by researchers coming from industry, such as S. Beyer (Global Foundries), S. Slesazeck (NaMLab gGMBH); J. Friis (SINTEF), D. Stewart (Western Digital), D. Gao (Nanolayers Research Computing LTD) along with our partners J. Ocker (Ferroelectric Memory

GmbH), S. Clima (Imec), and A. Padovani (AMAT). Speakers from EPFL, CNR, and ICN2 completed the dissemination by partners. Moreover, the workshop offered the stage to the project to present for the first time an IM2D demonstrator, which was a great success for its innovativity. M. Bülscherberger (Fraunhofer IWM), M. Bertocchi (AMAT), and F. dos Santos (EPFL) presented a demo to the public showing the complete, though initial, running of IM2D. A beta version of IM2D platform is available for early adopters.

A poster session, in which several postdocs from the project presented their work, completed the scientific programme.

COMMUNICATION KIT. The workshop had a dedicated website (https://intersect-workshop.icn2.cat/), designed by the ICN2 partner, still available and reachable from the Intersect website. The full programme, the agenda, the book of abstracts[1] and the videos of the talks can be found on the website. A promotional campaign was done on social media, on the partners' institutional websites, and through other websites. The communication campaign and the organizing committee was led by Mara Di Berardo, CNR, with the support of Alex Argemì, ICN2, and relative groups.

PROMOTION. The workshop has been promoted on several online channels.

Consortium media:

- CNR Nano website[2]
- Fraunhofer IWM website[3]
- Imec[4]
- ICN2[5]
- Applied Materials It LinkedIn[6]
- EPFL/MARVEL socials

Mailing lists and newsletter: CNR Nano; Unimore; Imec extranet; MaX CoE; ICN2

Other channels and websites:

- EMMC website[7]

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[1] https://intersect-workshop.icn2.cat/docs/INTERSECT-book-of-abstracts2.pdf

[2] http://www.nano.cnr.it/?mod=new&id=485 28/09/2021

[3] https://www.iwm.fraunhofer.de/en/aboutus/events/intersect-workshop.html

[4] https://www.imec-int.com/en/events/intersectworkshop

[5] https://icn2.cat/en/events/eventdetail/1714/intersectworkshop

[6] https://www.linkedin.com/posts/appliedmdlx%E2%84%A2-simulation-software_synapticelectronics-synapticelectronics-activity6848561491927465985-doiz

[7] https://emmc.eu/events/intersect-workshop-nov2021/

- Cordis website[8]
- Psi-k mailing list[9]
- CNR website[10]
- First ART-ER newsletter[11]; Rete Alta TEcnologia Regione E-R (LinkedIn group)[12]; First ART-ER website[13]; Emilia-Romagna Open Innovation Platform[14]

IMPACT. A total of 147 people registered for the workshop, and of these, 94 people actually attended, 26% coming from industry and 72% from research. The participants were from 8 EU countries (67 people) and from 15 extra-EU countries (27). Among them, we point out that two members of the AEB attended the conference.

PARTICIPANTS	Session 1 Nov. 10, 2021	Session 2 Nov. 11, 2021	Session 3, Nov. 11, 2021	Session 4, Nov. 12, 2021
In-person	31	27	29	27
Online	43	26	30	24
Total	74	53	59	51

Table III: Attendance of sessions.

The workshop website was launched at the end of September 2021: 857 unique users visited it in 1811 sessions, with a mean number of 3,6 pages viewed per session. 18 videos of the presentations have been uploaded in the ICN2 YouTube Channel[15] and are still available. They have gained so far 1232 views.

As for the INTERSECT social media, there was an intense preparatory activity from the launch on 27/09/2021, covered on Twitter by 23 tweets on announcement, agenda, speakers, followed by a live reportage of the event by 45 tweets about the program, the talks. A follow-up set of 9 tweets concluded the coverage, up to 20/12/2021 when the link

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[8]https://ec.europa.eu/info/events/internationalworkshop-advanced-materials-device-solutionssynaptic-electronics-2021-nov-10_en

[9] https://psi-k.net/events/international-workshop-onadvanced-materials-to-de/

[10]https://www.cnr.it/en/event/17495/international-workshop-on-advanced-materials-to-device-solutions-for-synaptic-electronics

[11]https://first.aster.it/_aster_/myFirst?data=2021-10-07&userId=6a292c4b2c5044c4cc415ebee62eee5fe5c28d12&utm_source=nl20211007&utm_medium=mail&utm_campaign=aster#myl

[12] https://www.linkedin.com/feed/update/urn:li:activity:6849615658292920320

[13]https://first.aster.it/_aster_/viewNews/52657/elettronica-e-calcolo-workshop-su-materiali-avanzati07/10/2021

[14] https://emiliaromagnaopeninnovation.aster.it/news/news/view?id=79301/10/2021

[15] https://www.youtube.com/playlist?list=PLav_yj0i6GkyQB-mi1j409X-QMU24bGqi

to available videos was shared. Similarly, on Instagram a total of 61 posts covered the event from announcement to last communication, and 34 on LinkedIn. During the conference, Twitter earned 2.8K impressions per day, a very high number for the account.
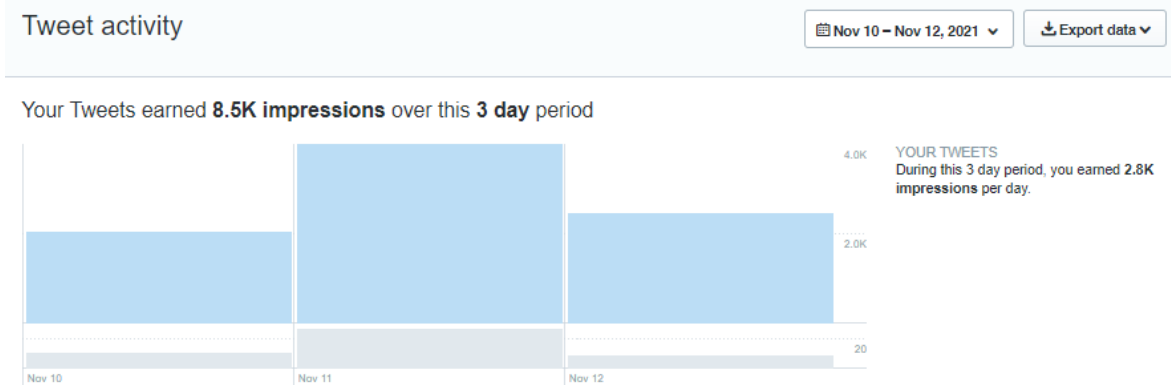

Figure 3. Tweet activity during the conference.

CONCLUSIONS. The workshop brought together experimental and theoretical experts in the field of electrical engineering, physics, chemistry, and materials science to discuss the main open problems and solutions for the development of volatile and non-volatile memories and memristors. A transversal interest emerged on the need to control the

Figure 4. (left) The workshop group picture; (right) P. Ordejòn (ICN2) and A. Calzolari, co-chair of the workshop.

operation power, and the cost of moving data through in-memory computing solutions, so as to face the energy challenge and reduce the carbon impact of digital systems. Taking advantage from the presence of leading experimentalists in the field, we systematically ask for the most urgent problems for them to solve in order to boost the advancement of their specific technology, and how modelling could help their research. Particular attention was

dedicated to materials-device codesign and to innovative interoperable automatic workflows for industry-driven applications, in close connection with the experimental side. It was an excellent way to discuss topics of interest of the project that went beyond the dissemination of project results. It was a self-standing event with well-known scientists and researchers discussing cutting-edge subjects.

3.2 The TechCafé "Combining semantic web technologies with automated workflows within the IM2D simulation tool box" - online, March 29, 2022

Figure 5. The TechCafé banner.

WHAT. A second event conceived for a specialized public, with special attention to the industrial audience, has been the **TechCafé "Combining semantic web technologies with automated workflows within the IM2D simulation tool box".** Organized mainly by the Fraunhofer IWM node with EPFL, this hands-on tutorial was meant for developers, ontologists, and MarketPlace users to gain insight into the technical architecture of an open simulation platform. EPFL and Fraunhofer IWM made the introduction to the fundamental technologies of AiiDA and SimPhoNy, which are the driving softwares in IM2D. Furthermore, the capabilities and app architecture of the IM2D REST API were explained in detail. These were supported by Jupyter-Notebook tutorials which were presented live. The overall purpose of these examples was to demonstrate the benefits of ontology-based technologies managing the persona profiles of IM2D through SimPhoNy in combination with the powerful workflow management of AiiDA. It was held online on March 29, 2022, from 10.00 to 11.30 CET.

HOW. During the tutorial, IM2D-toolbox and underlying technologies developed within the INTERSECT project were presented, through the applications code architecture and logics behind the ontologies applied in the interaction between SimPhoNy and AiiDA. The TechCafé was filled with practical API examples, hands-on tutorials, detailed explanations, and open discussions. The webinar was introduced by a welcome speech by our PI A. Calzolari, followed by an introduction to AiiDA by F. Dos Santos (EPFL), an introduction to SimPhoNy by J. Manuel Dominguez (Fraunhofer IWM), and then a talk on IM2D architecture and API by M. Büschelberger (Fraunhofer IWM). During the meeting the participants had the chance to gain further insight into the interoperability framework of IM2D based on the standards of the EMMO and DCAT. The API-tutorials showcased how the HTTP-resources provided by the ofREST services of IM2D can be facilitated by any arbitrary client, such as, e.g., under the hood of the graphical user interface which was developed by AMAT during the scope of this project. The handling of the GUI itself was not presented, since this was going to be the focus of the IM2D industry webinar, to be held on April 27, 2022.

COMMUNICATION KIT. The workshop had a dedicated website[16] designed by the Fraunhofer IWM partner, that is still available and reachable also from the Intersect website. A promotional campaign was done on social media, on the partners' institutional websites, and through other websites. The communication campaign was led by the ICN2 group that prepared a communication kit for the partners.

PROMOTION.

- Fraunhofer IWM website[17]
- EMMC website[18]
- Mailing lists: Cnr Nano, Unimore, MaX CoE, Fraunhofer IWM, EMMC, AFLOW community.
- Intersect twitter (4 posts from 18/3/2021 to 29/032021); 1 retweet by MaX CoE.
- LinkedIn: Intersect (2 posts), MaX CoE (1 post).
- Yambo-code.org Forum (1 post)

IMPACT. The TechCafé was attended by 35 participants (out of 51 registered people). The highest bunch was from Germany, followed by other four European countries and 6 non-European countries. The audience was consistently composed of academic researchers. Intersect tweets got globally 1430 impressions and 34 engagements.

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[16] https://www.iwm.fraunhofer.de/en/about-us/events/online-workshop-techcafe.html

[17] https://www.iwm.fraunhofer.de/en/about-us/events.html

[18] https://emmc.eu/events/intersect-techcafe-29-03-2022/

CONCLUSIONS. The TechCafé was conceived by the groups within INTERSECT that develop the IM2D tool. This format offered an excellent opportunity to present IM2D from a more technical point of view, and perfectly integrated with the other events about the toolbox. The hands-on experience was highly appreciated by the audience. Further private messages from workshop participants requesting access to the workshop material were subsequently incoming at the workshop coordination.

3.3 The "IM2D webinar: Presenting the simulation box for disruptive electronics" online, April 27, 2022

Figure 6. The IM2D webinar banner.

WHAT. As a final event for our project and a major means of dissemination of our IM2D toolbox towards industry and interested stakeholders, we organized a webinar aimed at explaining what IM2D is about and what it can offer. The process toward the actual event was quite long, as we wanted to prepare a useful event and to contact the widest possible audience. The **"IM2D webinar: Presenting the simulation box for disruptive electronics"** was broadcasted online on April 27, 2022 and introduced the IM2D platform main features through real application cases.

HOW. The webinar was organized by the whole consortium, with a special effort by ICN2 (that managed the content and technical supervision) and by participants from CNR and AMAT. The agenda provided an introduction about the project by PC A. Calzolari, followed by two speeches about "The challenge" (L. Larcher, AMAT) and "The answer" (P. Ordejon,

ICN2, and L. Larcher, AMAT). Then the three speakers interacted in a lively Q&A session. The second half of the webinar was devoted to a live demo of the IM2D simulation platform and was the core of our presentation to industry. We showed what the toolbox could do for tentative stakeholders, what its characteristics are, how it is usable also by non-experts, and what advantages it offers in materials development. Several questions from the public were answered at the end, about the beta-version of IM2D, of the need of HPC power to compute, or DFT calculations.

Figure 7. Images from the IM2D webinar.

COMMUNICATION KIT. A special page for the webinar was drafted within the Intersect website[19]. It showcased all the relevant information and was the gateway for registration. ICN2 communication group prepared a communication kit for the partners to use: a piece

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[19] https://intersect-project.eu/im2d-webinar/

of news to share on partners' websites, graphic cards to use on social media, a text for mailing lists.

PROMOTION.

- INTERSECT website[20]
- EMMC website[21]
- CNR NANO website[22]
- CORDIS website[23]
- Psi-K website[24]
- CNR website[25]
- ICN2 website[26]
- MAV (Materials Advancat de Catalunya) website[27]
- Mailing lists: Imec digital Bulletin Board (~5000 researchers); Cnr Nano, Unimore; Psi-K; EMMC.

Social media:

- Intersect social media: 10 Twitter posts, 5 linkedIn posts, 3 Instagram posts.
- LinkedIn post Amat (Applied-MDLx), Cluster MAV.
- Twitter posts by Quantum Espresso Foundation (QEF), PsiK, Cluster MAV, ICN2.
- Facebook post by QEF.

IMPACT. A total of 103 people registered for the webinar, and of these, 45 people attended, 10% coming from industry (e.g., Samsung, Tetrapak, Bita QUantum AI, Simune), 86% from research, and 4% coming from other sources. The participants were from 6 EU countries (46 people) and from 22 extra-EU countries (57). Among them, we point out that a member of the AEB attended the webinar.

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[20] https://intersect-project.eu/im2d-webinar/

[21] https://emmc.eu/events/intersect-im2d-webinar/; https://emmc.eu/news/intersect-im2d-webinar-apr-27-2022-1400-cet-new-date/

[22] https://www.nano.cnr.it/eventi-cnr/presenting-the-simulation-box-for-disruptive-electronics/

[23] https://ec.europa.eu/info/events/intersect-im2d-webinar-2022-apr-11_en

[24] https://psi-k.net/events/intersect-im2d-webinar/; https://psi-k.net/events/intersect-im2d-webinar-postponed-to-april-27-20/

[25] https://www.cnr.it/it/evento/17753/presentazione-di-im2d-la-simulation-box-per-una-nuova-elettronica

[26] https://icn2.cat/en/events/eventsbyyear/2022/48

[27] https://www.clustermav.com/esdeveniments/webinar-presentacio-de-la-plataforma-de-simulacio-per-a-electronica-disruptiva/

The IM2D page on the Intersect website since has been hit 2450 times (up to 28/04/2020) and has been the second most visited page of the whole website in the last month (761 visits).
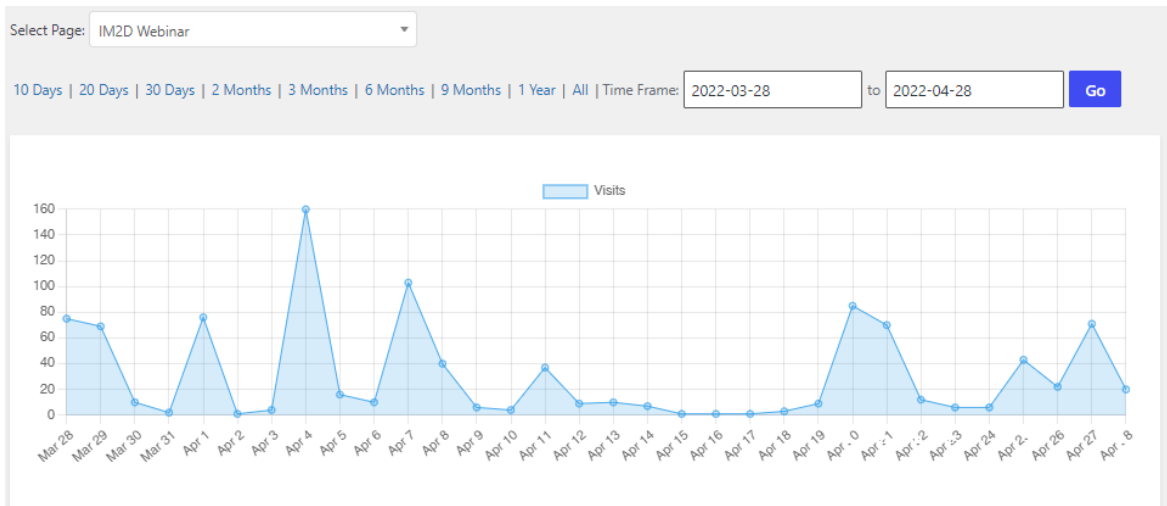

Figure 8. IM2D page on INTERSECT website statistics (up to 28/04/2022).

The 9 related Twitter posts (7 pre-event and 2 live) have reached a total of 4456 impressions and 148 engagements. The 5 LinkedIn posts have reached 565 impressions and an average engagement rate of 9.3%. The webinar has been recorded and is going to be public. We will continue with the promotion and hopefully reach out to a larger audience.

The webinar will be available on ICN2 YouTube channel, and we will continue to promote it as a gateway to IM2D for potential users. The survey submitted at the end of the webinar showed a high satisfaction level and demonstrates that the scope and the innovation of the toolbox has been well understood. For example, out of the respondents (11), 63% strongly agree and 37& agree with the sentence "IM2D INNOVATION: IM2D is an innovative and attractive tool"; 55% strongly agree that "IM2D BUSINESS: IM2D responds to research /market needs".
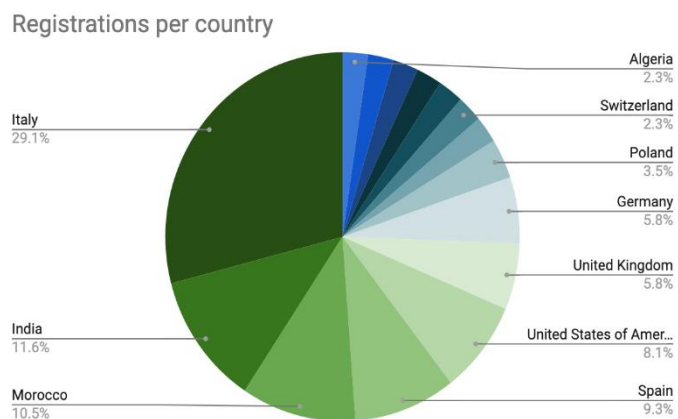

Figure 9. Countries of provenance of webinar registered users.

CONCLUSIONS. This webinar has been broadcasted at the very end of the project, also for some technical problems that obliged us to postpone the original date of April 11, 2022. Instant feedback from participants was very positive and in line with the interest expressed by the early user survey reported in D3.6. IM2D has almost come to completion, and we were able to present a running toolbox to the public. The software and the GUI are well functioning, and we definitely convey to the public the importance of this exploitable result of ours: an end-user can, from their laptop, calculate a set of properties of materials thanks to a user-friendly interface.

4.   Communication channels

A wide description of the communication tools was provided in D4.4. As no main changes occurred, we will present here the activity in RP2.

4.1 Website

The website (http://www.intersect-project.eu) has been conceived and designed as the most institutional of the Intersect media. It showcases the project as a whole and all related topics and news.

The home page as a stripe structure (news, people, contact details) and all internal pages are accessible from the upper right menu:
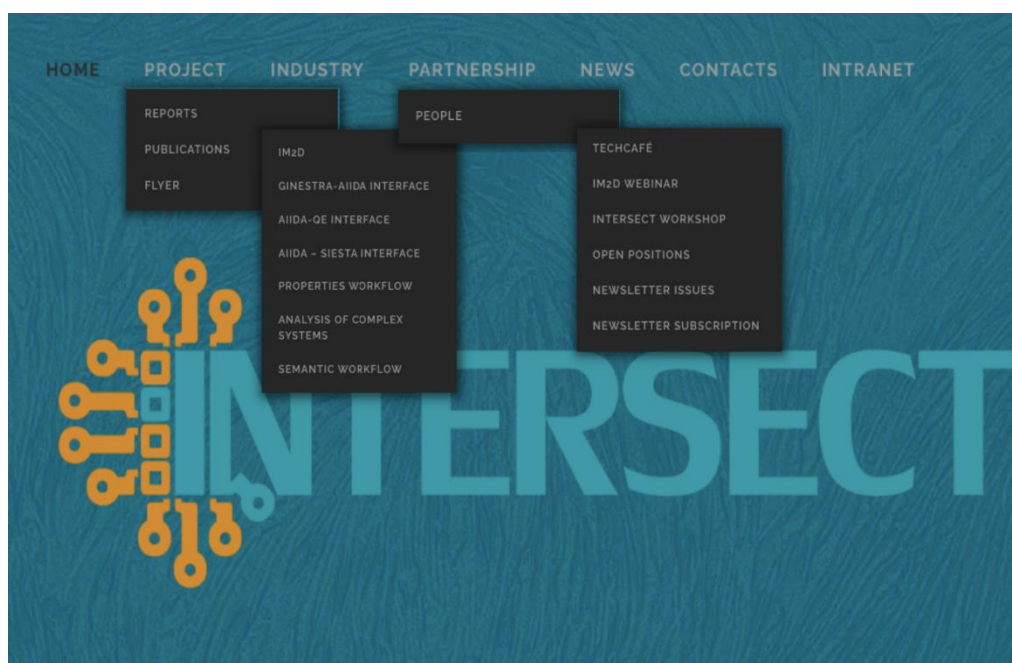

Figure 10. The structure of the INTERSECT website with open menus.

Two sections have been of paramount importance in the last months:

Industry (https://intersect-project.eu/industry/). In this section all the advanced solutions for industry-driven research are presented, via detailed descriptions, images, and videos. All items are also presented in downloadable .pdf format, with main product details at a glance. The exploitable results derive from the innovation activity of the consortium, as explained in D4.7 and D4.8. The list of results comprises:

- IM2D – Interoperable Material-to-Device
- Ginestra-AiiDA Interface
- AiiDA-QE Interface
- AiiDA-SIESTA Interface
- Properties Workflow
- Analysis of Complex Systems
- Semantic Workflow

-

Figure 11. Examples of "Product details" sheet, downloadable from the website.

News. Seventy-five pieces of news have been published in the addressed period. They have been usually also posted in social media, in a tailored way, and have regarded all fields of interest of the project: from job offers to new publications, to events. In particular, in the last months this section has been used to host sister websites or special webpages for the main events organized by the consortium, as IM2D events described above (see Chapter 3).

Impact. The website has had from M20 to M40 a total of 289.240 visits and 73.417 visits, With a peak of 5.588 visits on March 16, 2021 and of 1.184 visitors on November 28, 2020.
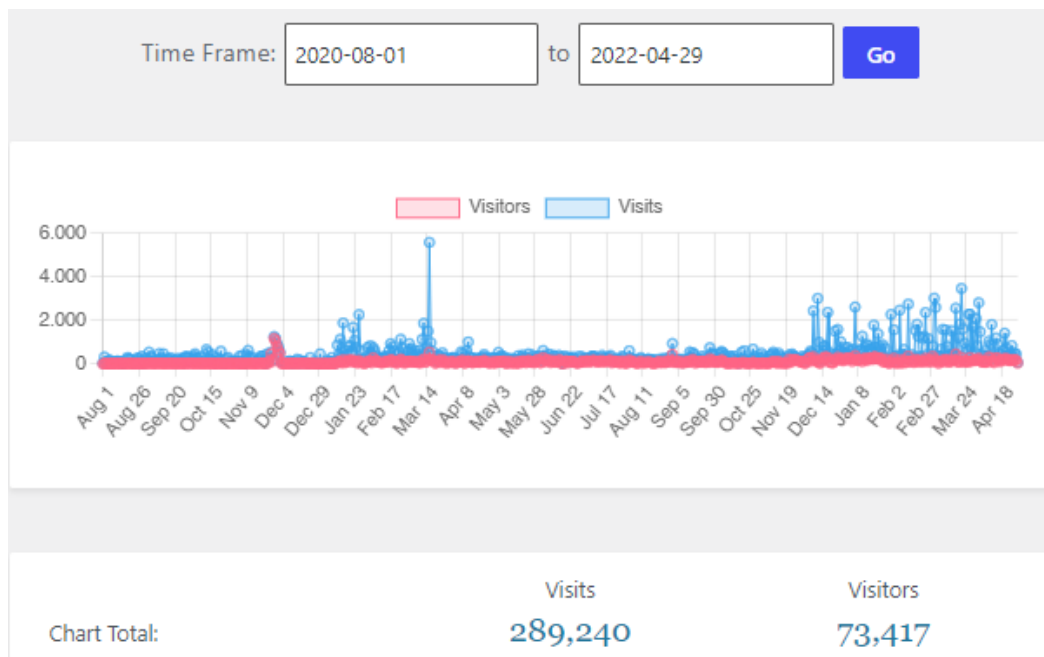

Figure 12. Website's hit statistics.

The provenance of visitors is displayed in the map below:

Figure 13. Map of INTERSECT website's visitors from countries of provenance

4.2 Social media networks

INTERSECT has used during its life three different social media, targeting messages to different audiences. The usage of social media permitted to share different contents, which would have probably been avoided in an institutional website, and to have more of a two-way kind of communication with the environment. From the project's point of view, Twitter turned out to be the most feasible one, as it is well established in the scientific community and among European projects. With the arrival of a communication expert at M19, who managed contents and posted regularly, we scored an increase in the follower numbers in all media.

Social media	Followers M1-M19 (RP1)	Followers M20-M40 (RP2) - growth rate)	Growth rate from RP1 to RP2
Twitter @intersect_eu	112	315	+181%
LinkedIn @intersect-project	51	176	+245%
Instagram @intersect_eu	58	183	+215%

Table IV. Number of followers at end RP1 and end RP2.

Main information and statistics related to the project social media channels are illustrated in the following sections.

4.2.1 Twitter

Figure 14. Twitter profile.

The Twitter account (https://twitter.com/intersect_eu) has been widely used during the project lifespan. Posting on Twitter gives the advantage of writing short text and adding images, flashcards, or videos, which makes the content more appealing. On the other hand, the medium is growing in the interest of the community (for example, many European projects have their own social media channels) but still it is difficult to build networks within followers. Nonetheless, our Twitter account

(@intersect_eu) has **315 followers** and an overall total of **632 tweets** have been written ranging on very different topics. We can list, among others: news about INTERSECT's life: people, deliverables, events, job opportunities, publications, internal meetings, etc, events of the INTERSECT partners, gender issues (see Figure 15), European political advancements, and much more. Moreover, we retweeted posts about topics of interest to the consortium and the community, e.g., news posted by other scientific and technological groups, or by EU projects and institutions, and high impact journals. A special effort has been done in covering live the main events of the last semester: the international workshop held in Barcelona (45 tweets during the event, 29 before and after it, see Chapter 3.1 for details) and the IM2D webinar (10 tweets, see Chapter 3.3 for details).

*Analytic*s. In months M20-M40 we posted **352 Tweets** that received 139K impressions (i.e., the times they were seen on Twitter), with an average of 219 impressions per month. We

Figure 15. Examples of Tweets about (upper left) Intersect-organized webinar; (upper right) a project meeting; (lower left) women-related event; (lower right) promotion of newsletter.

had 30 mentions and a growth of 203 followers (from 112 to 315). The followers come mainly from the research institution and academia sectors, then from other European projects. A good number of political institutions follow our account (e.g., @CORDIS_EU, the official CORDIS account, and @HorizonEU Official DG Research & Innovation account for EU's #HorizonEU research & innovation prog.).
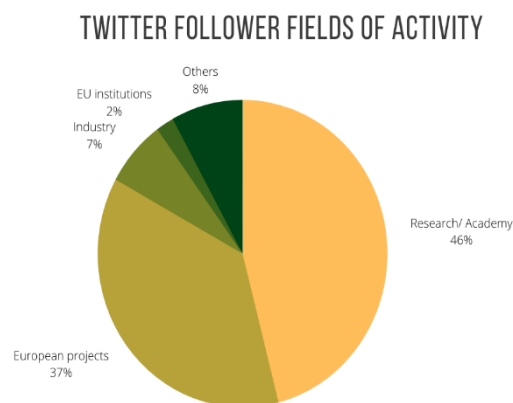
Data have been updated until April 27, 2022.

Figure 16. Followers sorted per field of activity.

4.2.2 LinkedIn

As it is well known, LinkedIn is a business-related social media platform. Our action on it (https://www.linkedin.com/company/intersect-project/) has therefore been more addressed to a scientific or an industry audience, with longer posts and participation to topic-related groups (e.g., Molecular Modeling in Material Sciences). A total of 279 posts have been published, ranging from Intersect related activities (open positions, deliverables, publications, events) to EU-policy related issues to events connected to INTERSECT people or topics.
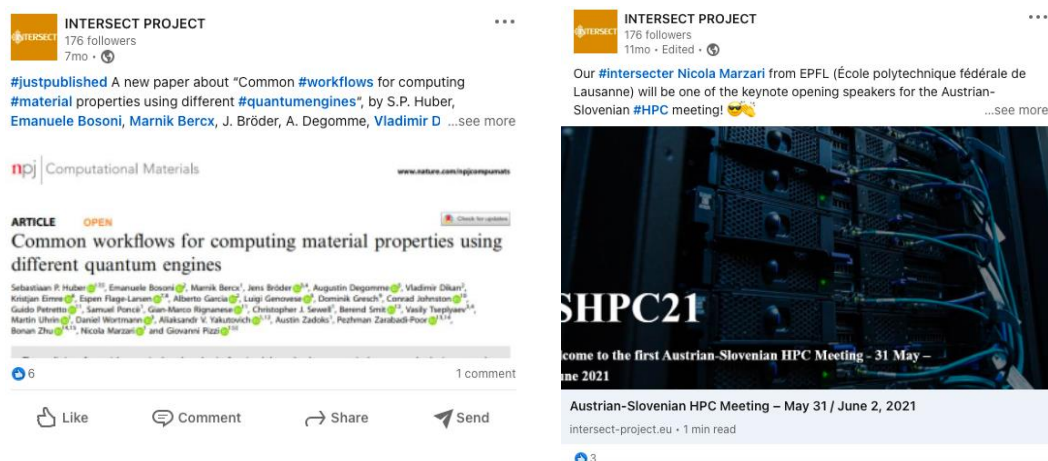

Figure 17 Examples of posts from the Intersect LinkedIn page.

In the last year we published **115 posts**, which got 15.963 impressions (24/04/2021-24/04/2022), 559 clicks and 346 reactions. The number of followers today is **176**, with an increase of 125 units with respect to reporting period 1.

The Follower Demographics presented in D4.4 have changed for the relevant growth of followers, and we want to point out here the change in the follower field of provenance. While in RP1 the total of followers from Research and Higher Education summed up to 59.12% of total (with a remaining 40.88% from Computer SW and HW industries, Nanotechnology, IT & Services, and others), now the sum of non-industrial followers is 48.8% (86 from Research, Higher Education, and Government administration) showing an increase in industrial followers of 10% (90 out of 176).
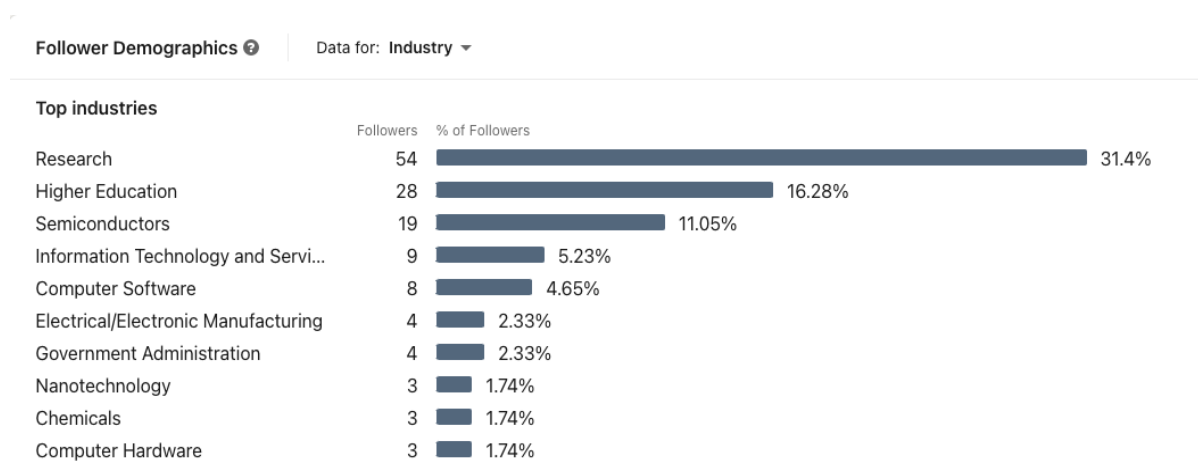
Follower Demographics ❓   Data for: **Industry** ▾

Top industries

	Followers	% of Followers
Research	54	31.4%
Higher Education	28	16.28%
Semiconductors	19	11.05%
Information Technology and Servi…	9	5.23%
Computer Software	8	4.65%
Electrical/Electronic Manufacturing	4	2.33%
Government Administration	4	2.33%
Nanotechnology	3	1.74%
Chemicals	3	1.74%
Computer Hardware	3	1.74%

Figure 18. Followers sorted per their field of activity.

Unfortunately, there are no available analytics for M20-M27, for the free version of LinkedIn supports data for just one year and no data for that period was stored by the communication officer, who left at the end of M37. Anyway, we had a growth in numbers from RP1 due to the hiring of the communication officer, and the average of posts, impressions, and engagement has been constant through the 2nd reporting period.

4.2.3 Instagram

A different approach has been used for Instagram. One of the most known social media for young people, it is not as flexible as Twitter for participating in discussion or does not have the same easiness in reposting or promoting others' contents. It is a media for sharing videos and images, which must therefore be prepared with the greatest care. Nonetheless, we built a small community there, reaching out to **183 followers** (+125 followers from RP1). We aimed to get in touch with the general public audience, fellow researchers or groups, in order to shed a different light on the project's results. Out of **240 posts** (only 7 in RP1), the most successful ones are those that show scenes of the work or meetings of the project people. Unfortunately, the limitations in travelling did not help this activity and led us to post contents more similar to those of the other social media channels.

Figure 19. A collection of the most successful posts from Instagram: all related to life scenes.

An analysis of followers is given below: they have been sorted into four groups for ease of assessment. Individuals, from scientists to co-workers to interested people, represent the widest group, followed by other European projects. Research and industry institutions are the last group, whether we have seen how active they are on Twitter and LinkedIn.
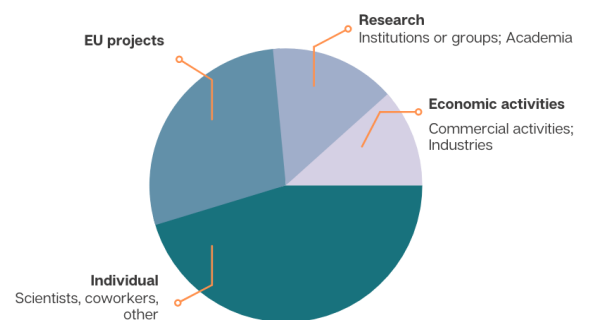
INSTAGRAM FOLLOWER PROVENANCE

Figure 20. Instagram followers sorted per kind.

4.3 Other activities

A list of other activities has been performed in RP2, that have a communication and dissemination purpose at the same time. We will present here the newsletter issues and the flyer draft.

4.3.1 Newsletter

As described in the communication plan, a newsletter was set up to reach out to different audiences about the major improvements and results of the project and to promote dissemination activities. The newsletter was sent to a dedicated mailing list of 112 contacts registered through the project website, collected during the previous dissemination activities or by promotion in the social media. The mailing activity has been performed using Mailchimp. After this specific activity the newsletters are permanently available for the general public on the project website at the dedicated page[28].

Figure 21. INTERSECT flyer.

Newsletter nr. 1 was issued on 12/03/2021 and presented the project, the IM2D toolbox concept, some selected publications, and upcoming events. Newsletter nr. 2 was issued on 17/03/2022 with the specific purpose of promoting the IM2D-related upcoming events, the TechCafé and the IM2D webinar.

4.3.2 Flyer

In the frame of communicating the scope of our project with the spotlight on our main result IM2D, in September 2021 we released a flyer in two versions: a poster, available on the website[29] for download in .pdf format, that offers an overview of the project and its advanced solutions for industry-driven research at a glance. The second reads the same content arranged in a threefold leaflet: It has been printed and sent to all partners for distribution to stakeholders and events.

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[28] https://intersect-project.eu/newsletter-issues/
[29] https://intersect-project.eu/flyer/

5. Dissemination activities

5.1 Seminars and Workshops

The partners disseminated the project's results and achievements through participation in conferences, workshops, events – mostly online ones - as invited or contributed speakers.

Below the list of the 36 talks (plus 5 posters) held in 21 events during RP2.

❖ **TechCafé - Combining semantic web technologies with automated workflows within the IM2D simulated tool box**, 29/03/2022, online:
- *José Manuel Domíngues* (Fraunhofer IWM), "Introduction to SimPhoNy".[30]
- *Matthias Büschelberger* (Fraunhofer IWM), "IM2D Architecture and API".[31]
- *Flaviano Dos Santos* (EPFL), "Introduction to AiiDA".[32]

❖ **IRPS Conference 2022**, 2022 IEEE International Reliability Physics Symposium - Tutorial & Year-in-Review Program, 27-21/03/2022, Dallas (US):
- *Ben Kaczer* (Imec), "Modelling ultra-fast threshold voltage instabilities in Hf-based ferroelectrics".
- *Ben Kaczer* (Imec), "Trap-polarization interaction during low-field trap characterization on hafnia-based ferroelectric gatestacks".
- *Andrea Padovani* (AMAT), "Reliability of non-volatile memory devices for neuromorphic applications: a modeling perspective", invited talk.

❖ *Nakib Haider Protik* (ICN2), "elphbolt: An ab initio solver for the coupled and decoupled electron and phonon Boltzmann transport equations" talk @ *APS March Meeting 2022*, March 15, 2022.

❖ *Amine Slassi* (CNR), "Tunable Schottky Barrier and Ohmic Contact at Interface Between TiN-Substate and Amorphous Materials" talk @ **International Conference on Current Trends in Advanced Materials and their Applications for Societal Development**. Online, March 8-10, 2022.[33]

❖ *Flaviano Dos Santos* (EPFL), "Magnetic excitations: From DFT to Model Hamiltonian", lecture @ **Ethiopian school on electronic structure methods and applications to**

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[30] https://www.iwm.fraunhofer.de/en/about-us/events/online-workshop-techcafe.html

[31] https://www.iwm.fraunhofer.de/en/about-us/events/online-workshop-techcafe.html

[32] https://www.iwm.fraunhofer.de/en/about-us/events/online-workshop-techcafe.html

[33] http://www.dhsgsu.edu.in/images/Downloads/conference-information.pdf

emerging energy technologies, College of Natural & Computational Sciences, Addis Ababa University (ET). Online, November-December 2021.

❖ *Roberta Farris* (ICN2), "Ab initio finite-temperature lattice dynamics calculations of thermal properties in TMDs materials" talk @ **Graphene Conference 2021**, Grenoble (FR). October 26-29, 2021.

❖ *INTERSECT* **International Workshop on Advanced Materials-to-Device Solutions for Synaptic Electronics**, November 10-12, 2021, hybrid (Barcelona and online):

Contributed talks:

- *Sergiu Clima* (Imec), "OTS material electrical parameter mapping from theoretical electronic structure Atomistic mechanisms for polarization switching and wakeup in HFOX-based Ferroelectrics".
- *Marnik Bercx and Flaviano José dos Santos* (EPFL), "Generating a FAIR crystal-structure database with the AiiDA informatics platform".
- *Johannes Ocker* (Ferroelectric Memory GmbH), "Interplay between polarization switching and charge trapping in ferroelectric field-effect transistors".
- *Matthias Büschelberger* (Frauhofer IWM), "SimPhoNy for ontology-based material exploration".
- *Andrea Padovani* (AMAT), "A Multiscale Approach to Identify Traps Responsible for Subthreshold Conduction and Threshold Switching in OTS Materials".
- *Nakib Haider Protik* (ICN2), "elphbolt - A free software for coupled electron-phonon Boltzmann transport".
- *Francesco Tavanti* (CNR), "Going deeper on the structural and electronic properties of amorphous GexSe1-x: a microscopic investigation".

Posters:

- *Luca Bursi* (CNR), "Ab initio characterization of defect states in materials for next-generation technology", poster presentation.
- *Arsalan Akhtar* (ICN2), "AiiDA Siesta Barrier: A workflow for high-throughput approach to diffusion in crystals".
- *Roberta Farris* (ICN2), "Lattice thermal conductivity of transition metal dichalcogenides".
- *Linda-Sheila Medondjio* (ICN2). "A-GeSe for selector materials: model preparation from first-principles".

- *Amine Slassi* (CNR), "Theoretical characterization of the Schottky/Ohmic contact between TiN-substate and amorphous materials".

❖ *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"**, November 1-3, 2021[34].

❖ *Flaviano Dos Santos* (EPFL), "Complex magnetic structure and spin waves of the noncollinear Mn5Si3", talk @ **Theos Group Meeting at EPFL**. Lausanne (CH), October 2021.

❖ *Nicola Marzari* (EPFL), "Digital infrastructures for materials discovery: the convergence of databases, simulations, and accelerators" @ **Virtual Materials Design 2021**. Online, July 20-21, 2021[35].

❖ *Arrigo Calzolari* (CNR), "INTERSECT latest advances" @ Special Workshop on EU projects (06/07/2021) during the **18th International Conference on Nanoscience & Nanotechnology (NN21)**. Thessaloniki (GR), July 6-9, 2021.

❖ *Nicola Marzari* (EPFL), "The Great Acceleration in Materials Discovery", invited speech @ **"Novel Materials Discovery – The Marvel of Computational Science"**, second edition of nexFrontier series by SwissNex. June 22, 2021 (online).[36]

❖ *Haidi Zhou* (FMC), "Mechanism of Retention Degradation after Endurance Cycling of HfO2-based Ferroelectric Transistors" @ **IEEE VLSI Symposium on Technology and Circuits.** June 13-16, 2021.

❖ *Nicola Marzari* (EPFL), "Materials discovery at the intersection between high-performance and high-throughput…" talk @ **Austrian-Slovenian HPC Meeting (ASHPC21)**. May 31 / June 2, 2021.

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[34] https://nomad-coe.eu/events/nomad-e-cam-workshop
[35] https://www.cecam.org/workshop-details/1093
[36] https://swissnex.org/china/event/nexfrontier-novel-materials-discovery-the-marvel-of-computational-science/

❖ *Nicola Marzari* (EPFL), "The great acceleration in the design and discovery of novel materials" webinar @ **"AI and ML in Materials Design and Discovery".** May 13, 2021 online.[37]

❖ *Nicola Marzari and Giovani Pizzi* (EPFL), "The AiiDA & Materials Cloud informatics platform for complex workflows" @ **"Simulation Workflows in Materials Modeling – SWiMM 2021"** workshop. March 15-26, 2021.[38]

❖ *American* **Physical Society (APS) March 2021 Meeting**, 15-19 March 2021, online:
  - *Flaviano José dos Santos* (EPFL), "Fermi energy determination for advanced smearing techniques"; 15/03/2021.[39]
  - *Francesco Tavanti* (CNR), "Amorphous Ge_xSe_{1-x} and its hierarchical structures by means of molecular dynamics simulations"; 16/03/2021.[40]
  - *Luca Bursi* (CNR), "Formation and diffusion of charged and neural defect states in crystalline GeSe for synaptic electronics"; 16/03/2021[41].
  - *Francesco Aquilante* (EPFL), "Accurate intercalation voltages for Li-ion cathodes from Hubbard-extended DFT" 16/03/2021.[42]
  - *Pablo Ordejón* (ICN2), "Addressing electrified metal-electrolyte interfaces with Non-Equilibrium Green's Functions" (by Ordejón and Febrer); 19/03/2021[43]

❖ *3rd* **EMMC international workshop 2021**, March 02/04, 2021 - online:
  - *Nicola Marzari* (EPFL), plenary talk about "The digital infrastructures for 21st-century science", March 3, 2021.[44]
  - *Arrigo Calzolari* (CNR), "IM2D: an industry-driven interoperable solution for the simulation-aided design of emerging electronics", March 2, 2021, talk + stand.[45]

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[37] https://bit.ly/3avgStB

[38] https://www.cecam.org/workshop-details/27#

[39] http://meetings.aps.org/Meeting/MAR21/Session/A20.3

[40] https://meetings.aps.org/Meeting/MAR21/Session/E59.5

[41] https://meetings.aps.org/Meeting/MAR21/Session/J53.10

[42] https://meetings.aps.org/Meeting/MAR21/Session/E61.5

[43] http://meetings.aps.org/Meeting/MAR21/Session/X19.1

[44] https://emmc.eu/emmc-2021/program/speakers/marzari/

[45] https://emmc.eu/emmc-2021/program/virtual_contribution/im2d-an-industry-driven-interoperable-solution-for-the-simulation-aided-design-of-emerging-electronics/

❖ *Flaviano Dos Santos* (EPFL), "Introduction to AiiDA. AiiDA tutorial", Lecture @ **University of ABC**, São Paulo (BR). February 2021.

❖ *Haidi Zhou* (FMC), "Application and Benefits of Target Programming Algorithms for Ferroelectric HfO2 Transistors" @ **IEEE International Electron Device Meeting.** December 12-18, 2020.

❖ *Adam Hashibon* (Fraunhofer IWM) invited speaker @ **"General Overview of European Virtual Materials MarketPlace Projects"**. September 30, 2020.[46]

5.2 Scientific Publications

The scientific publications listed below are the results of the scientific work performed during the entire project's life. Some publications were already listed in D4.4 in a preprint or submitted form.
Here, we report the complete list also available on the project's website with a link to the open access file (gold or green) to be compliant with the EU rules related to Open Access. Under each publication, if available, the metrics about Twitter or other media diffusion are given (thanks to Altmetric).

1. *Ovonic Threshold-Switching Gex Sey Chalcogenide Materials: Stoichiometry, Trap Nature, and Material Relaxation from First Principles*.
    S. Clima, D. Garbin, K. Opsomer, N. Avasarala, W. Devulder, I. Shlyakhov, J. Keukelier, G. Donadio, T. Witters, S. Kundu, B. Govoreanu, L. Goux, C. Detavernier, V. Afanasiev, G. Kar, and G. Pourtois. Physica Statu Solidi RRL 14, 1900672 (2020).
    DOI: 10.1002/pssr.201900672

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

    Altmetric: 13 tweets from 13 users, with an upper bound of 43,842 followers.

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[46]https://emmc.eu/events/materials-modelling-marketplace-vimmp-and-the-marketplace-overview-september-30-2020-1500-cest/

3. *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. Scientific Data 7, 300 (2020).
DOI: [10.1038/s41597-020-00638-4](10.1038/s41597-020-00638-4)

Altmetric: 12 tweets from 12 users, with an upper bound of 37,715 followers.

4. *Controlling the TiN electrode work function at the atomistic level*.
A. Calzolari and A. Catellani. IEEE Access 8, 156308-156313 (2020).
DOI: 10.1109/ACCESS.2020.3017726

5. *Hierarchical short- and medium-range order structures in amorphous GexSe1-x for selectors applications*.
F. Tavanti, B. Dianat, A. Catellani, and A. Calzolari. ACS Applied Electronic Materials 2, 2961–2969 (2020).
DOI: 10.1021/acsaelm.0c00581

Altmetric: 1 tweet from an account with 495 followers

6. *Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds*.
I. Timrov, F. Aquilante, L. Binci, M. Cococcioni, and N. Marzari. Phys. Rev. B 102, 235159 (2020).
DOI: 10.1103/PhysRevB.102.235159

7. *First principles investigation of charge transition levels in monoclinic, orthorhombic, tetragonal and cubic crystallography phase of HfO2*.
M. D. Nur K. Alam, S. Clima, B. J. O'Sullivan, B. Kaczer, G. Pourtois, M. Heyns, and J. Van Houdt. Journal of Applied Physics 129, 084102 (2021).
DOI: [10.1063/5.0033957](10.1063/5.0033957)

8. *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 Material Science 188, 110165 (2021).
DOI: 10.1016/j.commatsci.2020.110165

Altmetrics: 5 tweets from 5 users, with an upper bound of 4,013 followers.

9. *TB2J: A python package for computing magnetic interaction parameters.*
    X. He, N. Helbig, M. J. Verstraete, and E. Bousquet. Computer Physics
    Communications 264, 107938 (2021).
    DOI: 10.1016/j.cpc.2021.107938

    Altmetrics: 5 tweets from 5 users, with an upper bound of 17,125 followers.

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

    Altmetrics: 22 tweets from 21 users, with an upper bound of 43,695 followers.

11. *Giant Biquadratic Exchange in 2D Magnets and Its Role in Stabilizing Ferromagnetism
    of NiCl2 Monolayers.*
    J. Y. Ni, X. Y. Li, D. Amoroso, X. He, J. S. Feng, E. J. Kan, S. Picozzi, and H. J. Xiang. Phys.
    Rev. Lett. 127, 247204 (2021).
    DOI: 10.1103/PhysRevLett.127.247204

    Altmetrics: 7 tweets from 6 users, with an upper bound of 1,639 followers.

12. *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

    Altmetrics: 10 tweets from 9 users, with an upper bound of 37,879 followers.

News pieces:

-   The excellent heat dissipation properties of layered semiconductors revealed
    down to one layer (Phys.org, 01 Feb 2022).

- Thin is cool: researchers unveil the excellent heat dissipation properties of layered semiconductors down to the monolayer. (Nanowerk, 01 Feb 2022).
- Thin is Cool: Researchers Unveil the Excellent Heat Dissipation Properties of Layered Semiconductors Down to the Monolayer (Azonano, 01 Feb 2022).

13. *The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations.*
N.H. Protik, C. Li, M. Pruneda, D. Broido, and P. Ordejón. npj Computational Materials 8, 28 (2022).
DOI: 10.1038/s41524-022-00710-0

14. *BELLO: a script tool for bond element and lattice local-order analysis of disorder systems.*
B. Dianat, F. Tavanti, A. Padovani, L. Larcher, and A. Calzolari. Compt. Mater. Sci. 209, 111381 (2022).
DOI: 10.1016/j.commatsci.2022.111381

Altmetric: 2 tweets from 2 users, with an upper bound of 6,257 followers.

15. *A multi-technique approach to unravel the (dis)order in amorphous materials.*
F. Tavanti and A. Calzolari, submitted in ACS Omega (2022), in press.

More papers submitted or in preparation:

16. Device-to-materials pathway for electron traps detection in amorphous GeSe-based selectors.
A. Slassi, L. S. Medondjio, A. Padovani, F. Tavanti, S. Clima, D. Garbin, B. Kaczer, L. Larcher, P. Ordejón, and A. Calzolari. Manuscript in preparation (2022).

17. Formation and diffusion of point defects in crystalline GeSe.
L. Bursi, R. Chouhan, A. Catellani, N. Marzari, and A. Calzolari. Manuscript in preparation (2022).

18. Theoretical characterization of the Schottky/Ohmic contact between TiN-substate and amorphous materials.
A. Slassi, F. Tavanti, S. Clima, D. Garbin, B. Kaczer, and A. Calzolari. Manuscript in preparation (2022).

19. Fermi energy determination for advanced smearing techniques.
F. J. Dos Santos, and N. Marzari. Manuscript in preparation (2022).

5.3 Collaboration with other projects/EU ecosystem

A rich and fruitful activity of collaboration has been done within the European ecosystem. The participation in sister projects in the fields of ontology, workflows, open innovation platforms, standardization, has permitted a transversal dissemination of results. For example, as described in D5.3, the PC set up a synergic collaboration with the INTERSECT twin projects SimDOME and ReaxPro for the realization of a joint development team for EMMO implementation.

In the following, we give a list of such collaborations:

- Horizon 2020 twin projects SimDOME and ReaxPro.
- Horizon 2020 projects BIG-MAP, NFFA (Nanoscience Foundries and Fine Analysis), MarketPlace, OpenModel, MaX CoE, IQubits.
- EMMC: an organization promoting materials modeling with focus on industrial research and innovation. Initiated as a CSA, since 2019 it has evolved into the EMMC ASBL Association.
- OPTIMADE: The Open Databases Integration for Materials Design consortium to make materials databases interoperable by developing a specification for a common REST API.
- Psi-k network.
- NCCR MARVEL (CH).

5.4 Industrial uptake

As explained above, our activities have had in the last month a strong drive towards industrial uptake, and this will continue in the months to come. In the following we give a list of companies that have had contacts with INTERSECT thanks to communication/ dissemination activities or via members.

Company	Website address	Country
Bita Quantum AI		Canada
Global Foundries	https://gf.com/	USA/Germany
Goldbeck GmbH	https://www.goldbeck.de/	Germany
Ghorofa Technology Ltd		Kenia

IBM	https://www.ibm.com/uk-en?lnk=m	USA
Matgenix	https://matgenix.com/	Belgium
Materials Design, Inc	https://www.materialsdesign.com/	France
NaMLab gGmbH	https://www.namlab.com/	Germany
Nanolayers Research Computing LTD	https://www.nanolayers.com/	UK
NeoLogic vlsi	https://www.neologicvlsi.com/	Denmark
PWPW s.a.	https://www.pwpw.pl/en	Poland
Quantum ESPRESSO Foundation	https://foundation.quantum-espresso.org/	Slovenia
Robert Bosch GmbH	https://www.bosch.com/	Germany
Samsung	https://www.sait.samsung.co.kr/saithome/main/main.do	UK
Schrodinger Inc.	https://www.schrodinger.com/	USA
Simune Atomistics s.l.	https://www.simuneatomistics.com/	Spain
Synopsys	https://www.synopsys.com/	USA/Israel
Tetra Pak	https://www.tetrapak.com/	Switzerland
Western Digital	https://www.westerndigital.com/	USA
Air Liquide s.a.	https://www.airliquide.com/	France

Table V. List of companies that interacted with INTERSECT.

Conclusions

The pandemic in the last two years changed a lot our habits in work and social life, reducing the opportunities for interpersonal events to a very few, and promoting a online communication that may be effective, time saving, but lowers the to the minimum the interchange that is one of the benefits of events. Nonetheless, as a consortium we were able to timely carry on the project activities and the communication and dissemination ones as well. Luckily enough, we could hold our international workshop in Barcelona last

November in presence, with a tangible added value given by the proximity of speakers and public.

As detailed above, the activities we developed for the uptake of our results were manifold and various and were more planned. Online activities do not always permit us to collect feedback, but we will keep tracking some possible industrial uptake on the one side, and dissemination of scientific results on the other (e.g., with submitted publication).

As from articles 28 and 29 of the Model Grant Agreement, we will continue to exploit and disseminate the project results up to four years after the end of the project taking advantage of all EU tools, such as the Funding & Tenders portal and the Horizon Results Platform.