D3.6

Second report on IM2D box evaluation

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Version	Date	Modified by	Modification reason
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v.02	27/04/2022	Arrigo Calzolari	Final version

Content

[1] Acronyms are marked in purple in the text and defined at the end of the document.

1 Executive Summary

The present document is the deliverable D3.6 – "Second report on IM2D box evaluation through user feedback based on the FOMs", which is prepared under the Task 3.5. "Testing and user's feedback", as a part of Work Package 3 "Testing and piloting".

The main goal of the INTERSECT project has been the development of an industry-ready integrated, standardized, interoperable software platform called Interoperable Materials to Device (IM2D). IM2D integrates some of the most used open-source materials modelling codes, Quantum ESPRESSO (QE) and SIESTA, with models and modelling software for emerging devices (Ginestra®) via the SimPhoNy infrastructure for semantic interoperability based on ontologies, and powered by the AiiDA workflow engine, and its data-on-demand capabilities and apps interface. IM2D combines advanced software solutions that in principle would require users to have multi-disciplinary advanced skills (quantum mechanics, materials science, solid-state-physics, electrical engineering, informatics) to use it. However, the semantic level of interoperability along with the workflow automation are conceived to simplify the complexity of the problem and to make IM2D a user-friendly product, easy to install, browse and run, especially for industrial stakeholders.

The scope of Task 3.5 is to evaluate the IM2D box effectiveness during the project, enabling the continuous improvement of the platform well beyond the end of the project. The D3.6 report pursues the quality assessment guidelines defined in the D3.3[2]. In this regard, the survey proposed in D3.3 has been used to collect user's feedback. We first collected data from different user types (*persona*) as defined in D1.1[3]. The data are then analyzed in terms of the Figures of Merits (FOM) defined in D3.3, with the aim to quantify the performances and the quality of the results produced by the IM2D box, from the user's standpoint.

1.1 About this document

The aim of this deliverable is to analyze the user's feedback about the IM2D box effectiveness based on the D3.3 quality assessment framework and Figures of Merit, following the ISO/IEC 9126 standard. The First Section will briefly recap the D3.3 quality steps and FOM; the second section will be focused on the IM2D user profile analysis; the third section will analyze the user feedback results illustrating the main results for each step. Finally, the conclusion will compare the new and the previous (D3.3) results to evaluate the IM2D box effectiveness and its improvements during the project.

[2] https://intersect-project.eu/wp-content/uploads/2022/04/D3.3.pdf
[3] https://intersect-project.eu/wp-content/uploads/2022/04/D1.1.pdf

2 Quality Assurance Recap

In this section, we briefly recap the INTERSECT quality assessment framework and FOM established in the D3.3 based on the quality criteria coded in the ISO/IEC 9126 standard. This framework has been adopted in this deliverable to evaluate '*quality in use*' of IM2D on the basis of the user case and of the user profiles defined in the D1.1.

2.1 Figure of Merit (FOM)

To evaluate the IM2D quality standard, in D3.3 we proposed three main characteristics, namely **Functionality, Usability, and Maintainability**, and few of their sub-characteristics as those detailed in Table I.

Table I – Selected Sub-characteristics of the ISO 9126-1 quality model applied to INTERSECT (from D3.2)

INTERSECT FoM's	Description	Sub- characteristics	Explanations
Functionality (external)	In INTERSECT the functionality FoM analyzes how the IM2D meets project goals and user expectations. Interoperability is a key measure for checking the T2.1 and T2.3 status and a general goal of the overall INTERSECT project. At the same time, Suitability and Accurateness characteristics are important to check the Simulation hub outputs alignment with the User expectation. (In general, what the software does to meet needs)	Suitability Accurateness **Interoperability**	'Can IM2D perform the workflow/simulation required?' 'IM2D works as expected?' 'Can the platform interact with all the sub systems?'
Usability (external)	Usability is the key aspect for INTERSECT. IM2D will require a small effort for use thanks to its user-friendly and attractive Graphical User Interface (GUI). T1.4 is implementing a GUI for facilitating IM2D understandability and Operability.	Understandability Operability Attractiveness	'Does the user comprehend how to use the IM2D easily?' 'Can the user use the IM2D without much effort?' 'Does the GUI look good?'
Maintainability (internal)	In INTERSECT, IM2D Extensibility is essential to enable multiple software integration under a common platform. IM2D platform integrates widely used open-source materials modelling codes (Quantum ESPRESSO and SIESTA) with models and modelling software for emerging devices (Ginestra™) via the SimPhony infrastructure for semantic interoperability based on ontologies, powered by the AiiDA workflow engine,	**Extensibility** Flexibility	'Can the software be easily modified?' 'Can the software continue functioning if changes are made?'

	and its data-on-demand capabilities and apps interface. At the same time, the platform should be flexible to include corrections, improvements or adaptations.		

2.2 Quality framework

In D3.3, we defined a four-step protocol to test the IM2D quality, reported in Figure 1 for clearness. The quality framework starts from the direct experience from users, each attaining a specific use case and a *persona* profile (set-up). Users are asked to compile a survey where they indicate their opinions on their IM2D experience (collect-feedback). Data are then analyzed in terms of the FOM described above (feedback-analysis). Finally, data are used to change/improve IM2D (feedback-implementation).

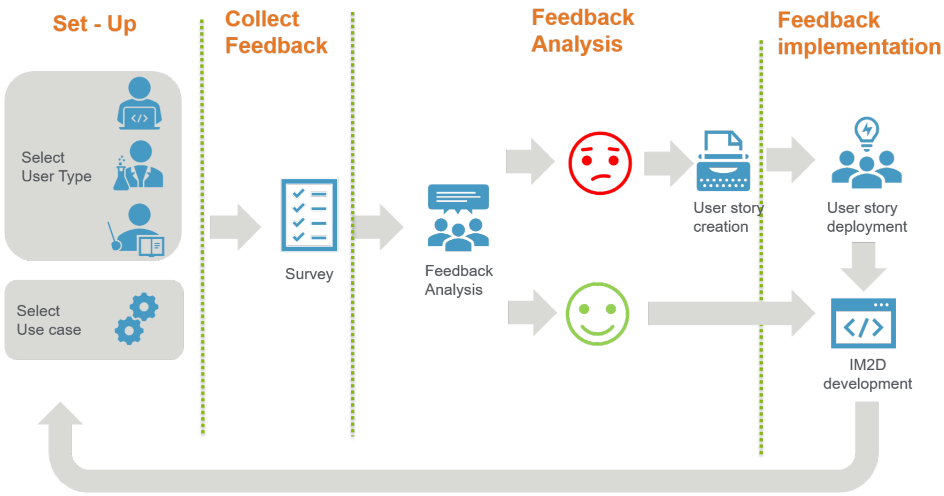

Figure 1. Quality Assessment Workflow (from D3.3).

3 Second Evaluation report

To elaborate the second evaluation report of the IM2D box we interviewed different target users corresponding to different *persona* profiles and we considered both material-to-device (M2D) and device-to-materials (D2M) use cases. In this way the target audience has been able to fully test the IM2D capabilities and provide useful feedback for a further development of the platform.

Note: user interviews were taken on an anonymous basis, no personal or confidential data of the interviewed people will be reported in this document that exposes only general information and aggregate results.

In the following, we will illustrate the evaluation steps following the Quality assessment framework depicted above.

3.1 Set-Up

In the Set-up phase we define the target audience and identify the use cases. The table below shows the Set-Up framework:

Objective:	Define the user target and use cases to set up the quality assessment
Input	User type and Use case in D1.1
Actions	- Define the use case to track. - Select the target user type based on the D.1.1
Output	Use case and user type target definition

3.1.1 User analysis

We target a pool of 55 early adopters with different *persona* profiles: 25 users from academia and 30 from industry (Figure 2). Users from academia correspond to *Persona #3*, users from industry have profiles from both *Persona #1* and *Persona #2*. The main characteristics of the persona profiles are summarized in Table II (from D1.1).

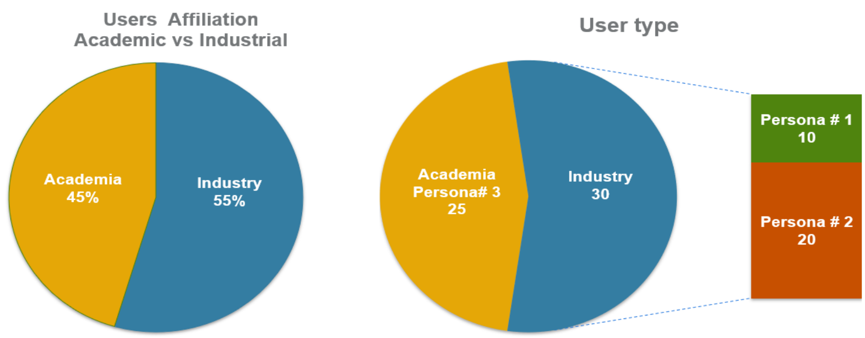

Figure 2. Second report's target user analysis

Table II - User type (definitions from deliverable D1.1, gray color). Number of users (black) divided in persona type.

User type	D1.1 Definitions	Affiliation	Role	# Users
	**Persona #: 1** Process engineer in a company, expert in the optimization/characterization of specific materials but with no experience/knowledge in	**Semi-Industry**	**Process engineer** **Electrical engineer** **Physicists** **Material scientists**	**10**

	device modelling (Aa2). This *persona* is the prototypical final user that will use IM2D as a black-simulation box.			
	**Persona #: 2** Engineer in a company, expert in the optimization/characterizatio n of specific devices but with experience/ knowledge in material (electronic/atomistic) models (Ab5).	**Semi-Industry**	**Device Engineer** **TCAD engineer**	**20**
	**Persona #: 3** Researcher from academy, with background in materials modelling, including electronic models, but with no experience/knowledge in device or circuit optimization (Bc17).	**University** **Research** **Center**	**Professors** **Researchers** **Post Doc**	**25**

3.1.2 Use Cases

Along the lines described in D3.3, we organized the use case evaluation session in 3 parts:

i. Brief introduction on IM2D.
By describing the IM2D box components and interconnections (Figure 3) the user has information about the necessary input/knowledge/parameters to perform the use case and evaluate the infrastructure.

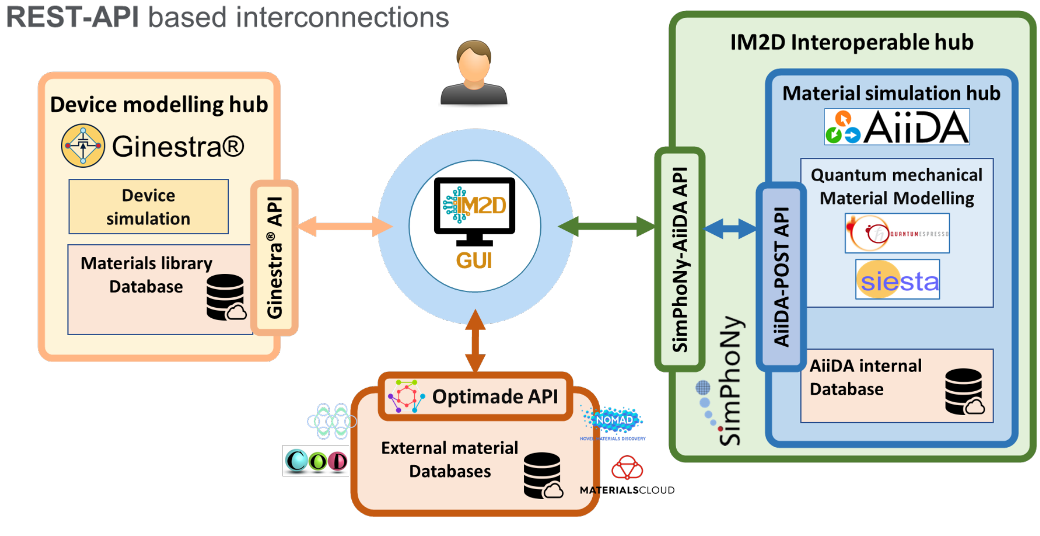

Figure 3. IM2D box components and interconnections.

ii. Material-to-device (M2D) use case.

The user performs one of the existing workflows for the evaluation of materials properties on demand (e.g., band gap, defect formation energy) to test the IM2D capabilities of optimizing the device characteristics starting from tailoring of the material properties and fabrication process effects (Figure 4).

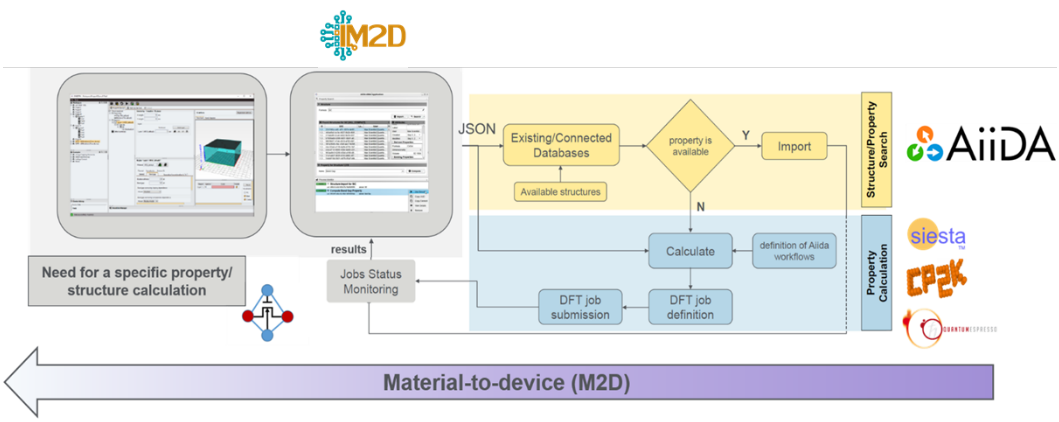

Figure 4. M2D workflow.

iii. Device-to-Material (D2M) use case.

Starting from the experimental electrical characteristics of the device, the user tests the IM2D capability of characterizing the atomistic properties of the new materials and new compounds, by using a multi-physics technique that combines defect discovery tools and quantum mechanical ab initio simulations (Figure 5).

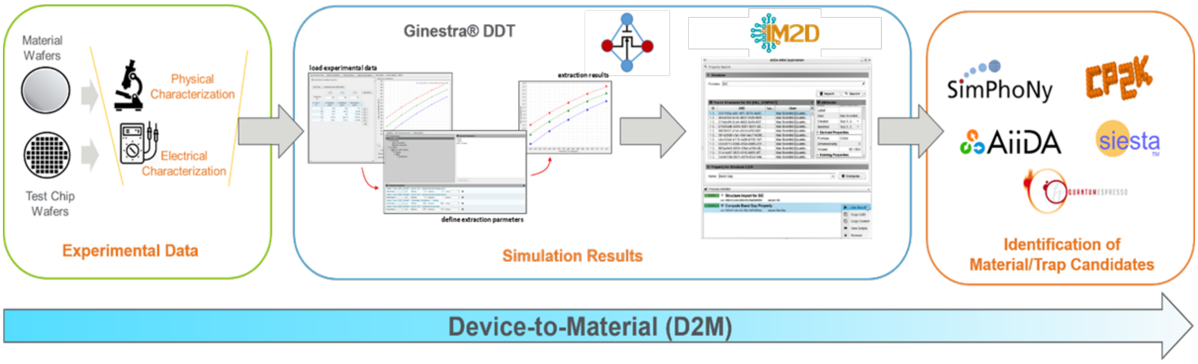

Figure 5. D2M workflow

These three parts are described in detail in the rest of the Section.

i. Brief introduction on IM2D

In the following we briefly summarize the main steps and the possible options the user runs into the IM2D use.

1. First IM2D Launch

At the very beginning, each user needs to configure the IM2D interface.
By launching the IM2D box, the splash screen shows the version and the INTERSECT partners that contributed to the IM2D box development (Figure 6).
In the windows bottom the user finds different tabs to configure their own settings

- ***About tab:*** it lists the INTERSECT credits (Figure 7)
- ***Preferences tab*** from which the user can:
    - select the look&feel settings
    - set the AiiDA connections
    - set the Symphony user expertise (ADVANCED, INTERMEDIATE, BASIC) which correspond to the persona profiles defined in D1.1:
        - BASIC is typically suggested to Persona #1
        - INTERMEDIATE is suggested to Persona #3
        - ADVANCED is suggested to Persona #2
    - Set the Material Project connection
    - Set the OPTIMADE connection
- ***AiiDA tab:*** the user can query Quantum ESPRESSO and Siesta directly through AiiDA framework (Figure 8)
- ***SimPhoNy tab:*** the user can exploit the SimPhoNy tools to retrieve the information from AiiDA, on the basis of their level of expertise (Figure 9)
- ***Material project tab:*** the user can query Materials Project database https://materialsproject.org/ (Figure 10)
- ***OPTIMADE tab:*** the user can exploit OPTMADE API to query multiple open material database https://www.optimade.org (Figure 11)
- ***Task Monitor tab:*** the user can monitor the status of the running jobs.

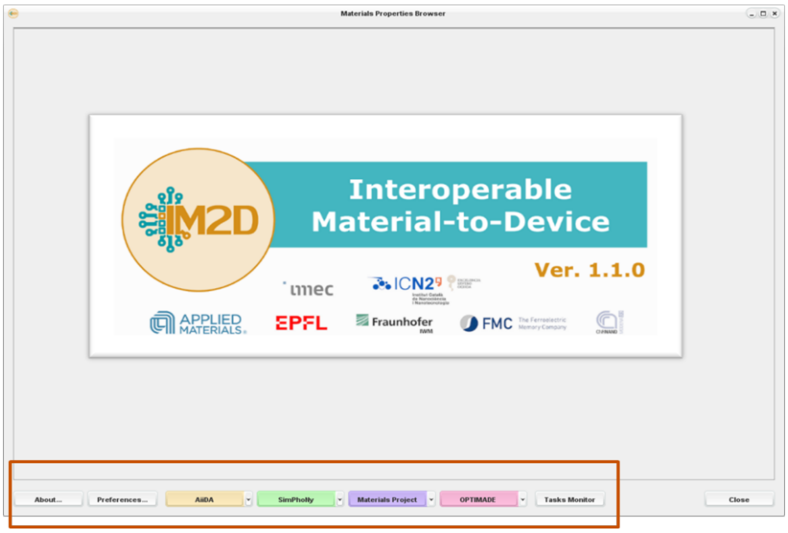

Figure 6. IM2D GUI main page.

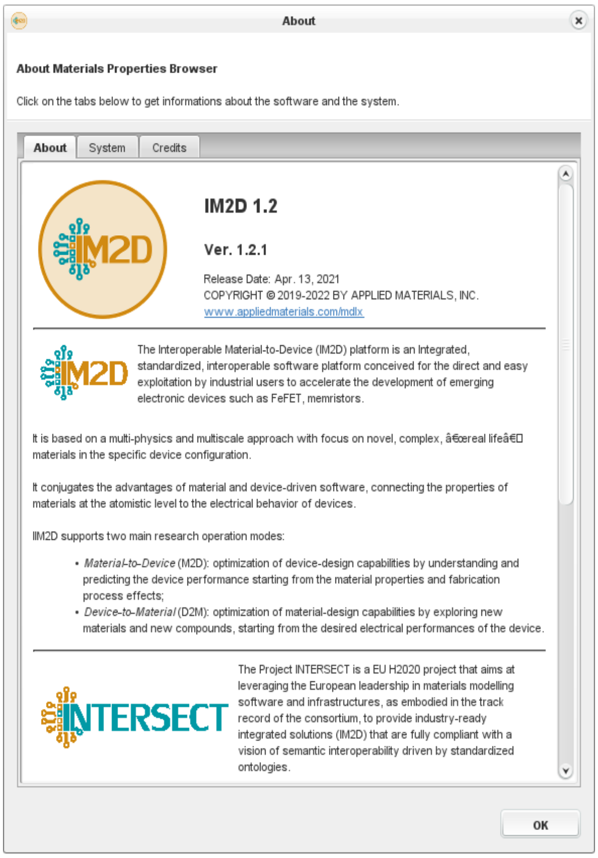

Figure 7. IM2D About tab.

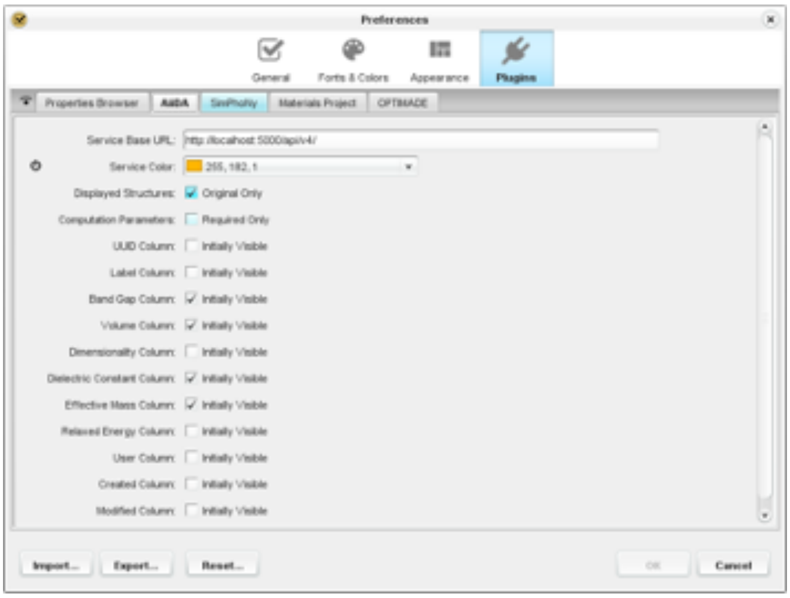

Figure 8. AiiDA settings.

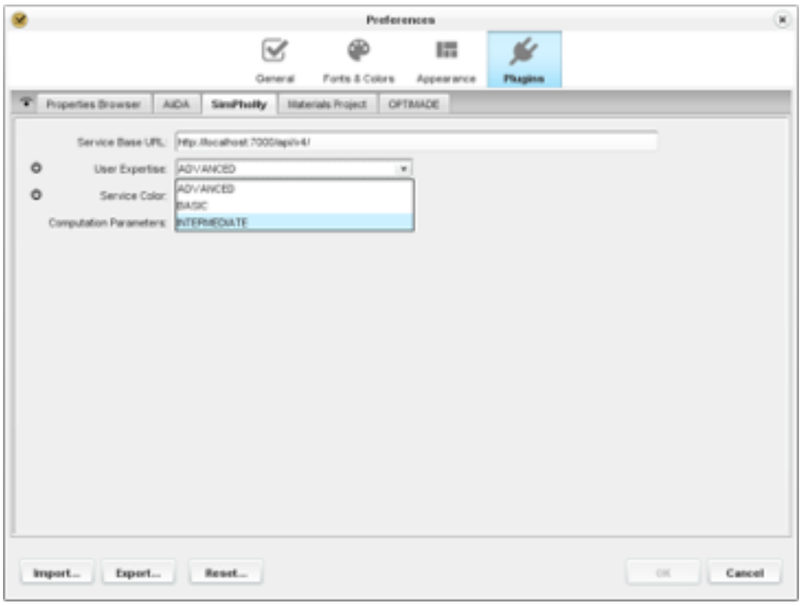

Figure 9. Symphony settings of persona profiles.

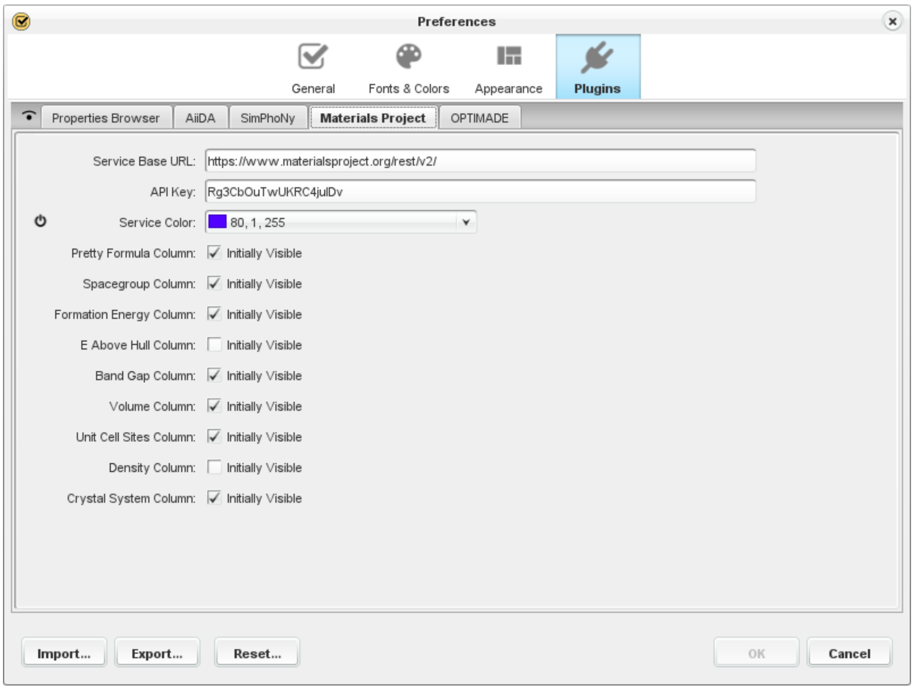

Figure 10. Materials Project settings.

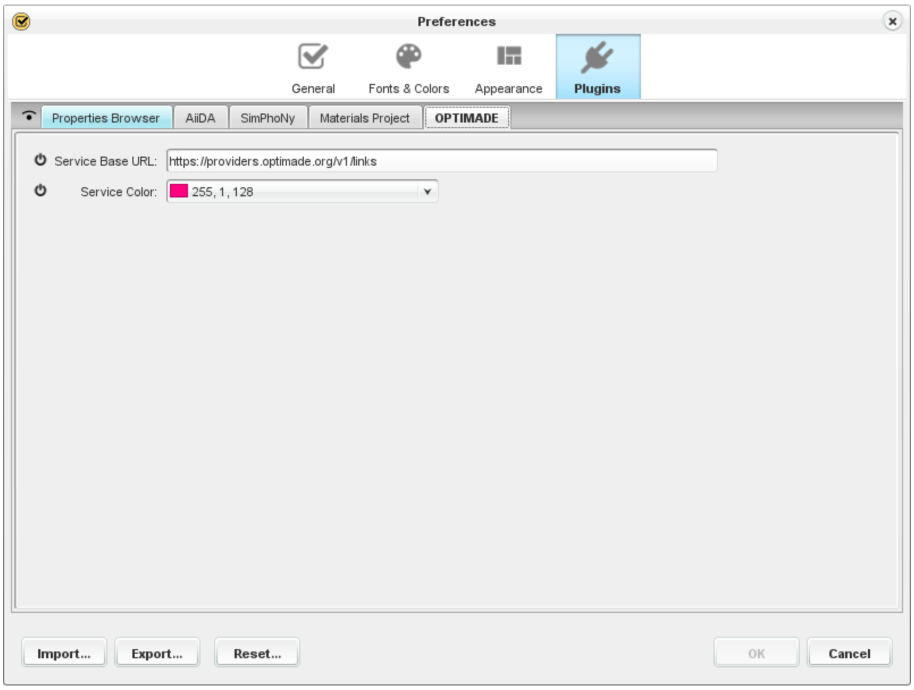

Figure 11. OPTIMADE Settings.

2. IM2D Basic Operations

- ### IM2D Database query

- Retrieve the list of structures using different filters and search options, for example by formula (Figure 12), by groups (Figure 13), or by chemical element (Figure 14)
- Opening a structure data page (Figure 15)

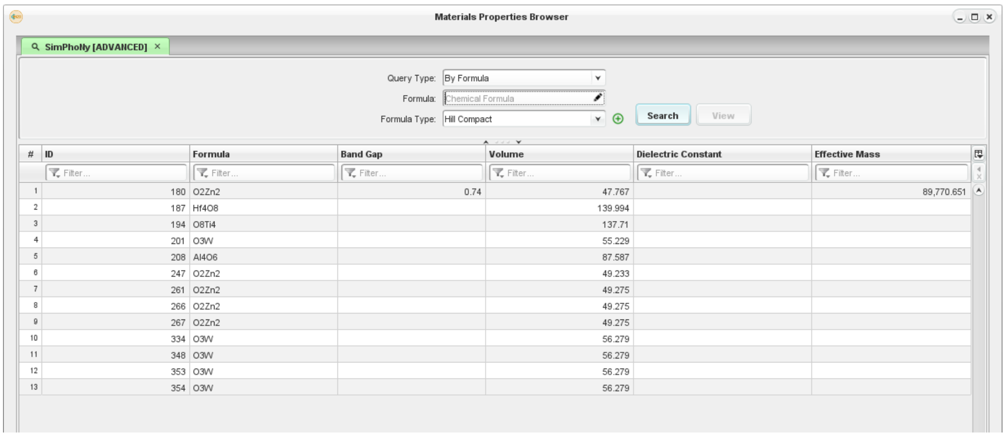

Figure 12. Materials data searching by Formula.

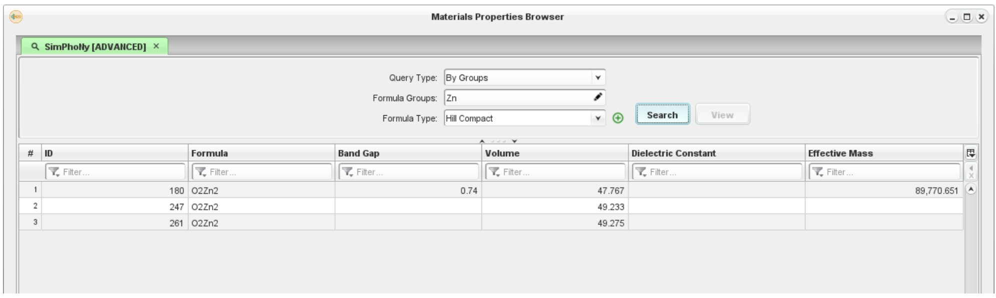

Figure 13. Materials data searching by Group.

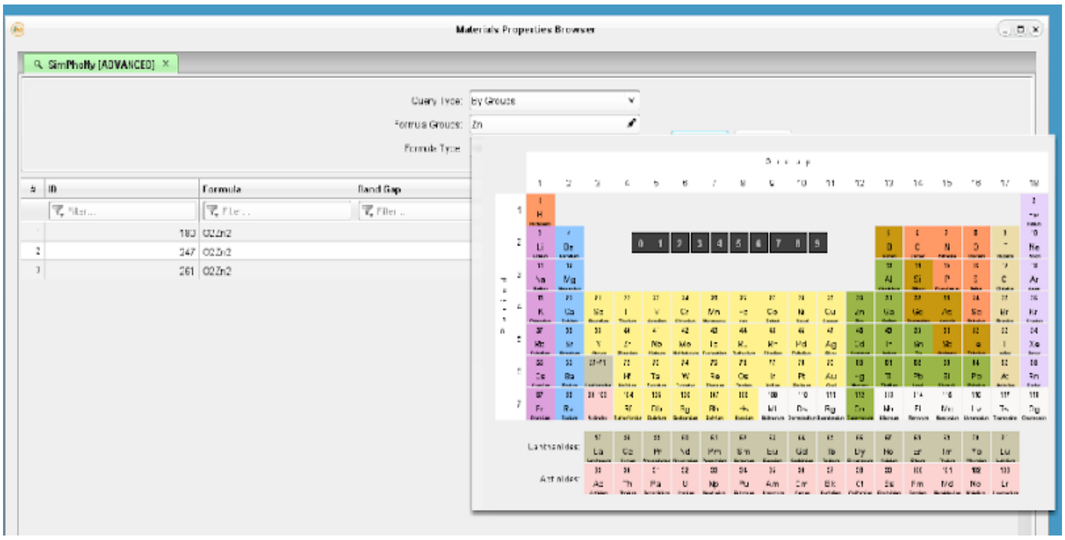

Figure 14. Materials Data searching using the periodic table.

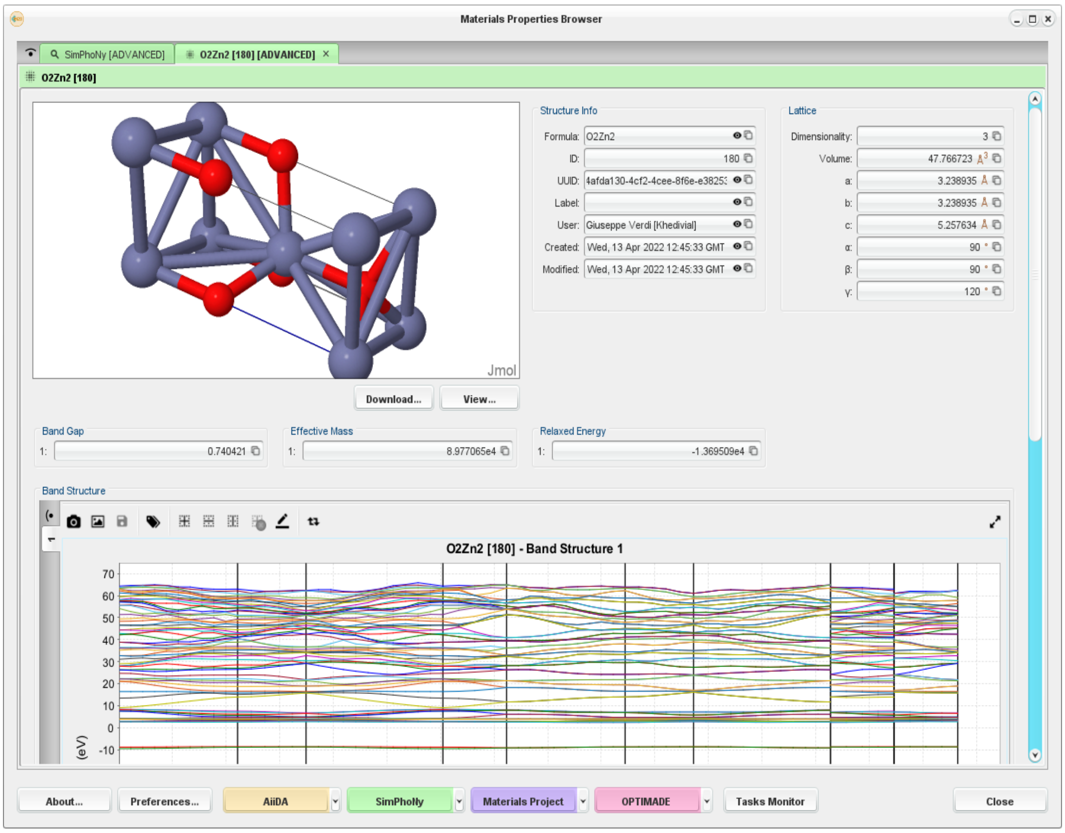

Figure 15. Open a Data Structure.

- **importing of a crystalline structure**
  - import a .CIF from databases (Figure 16)

- upload a .CIF structure from file list to be used as input structure for DFT calculations (Figure 17)

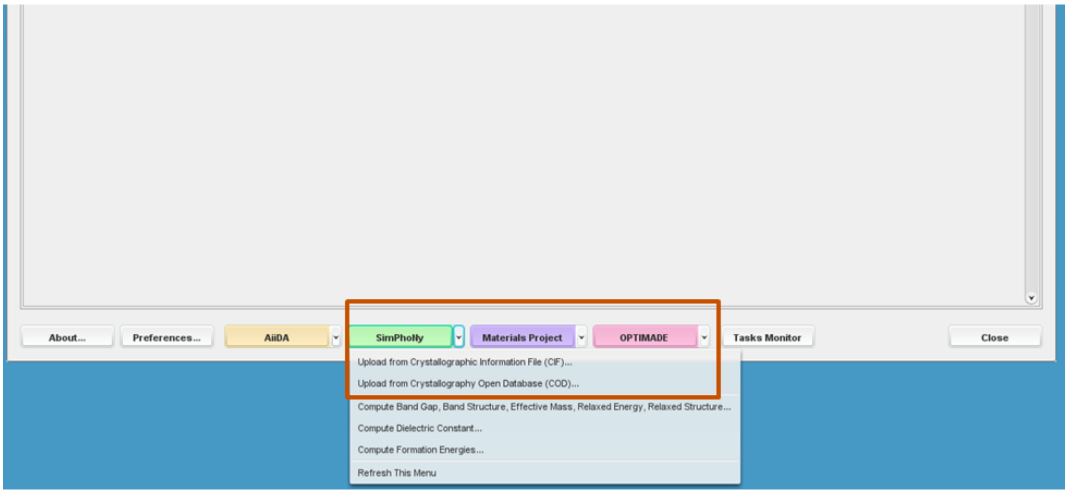

Figure 16. import a .CIF file from a database.

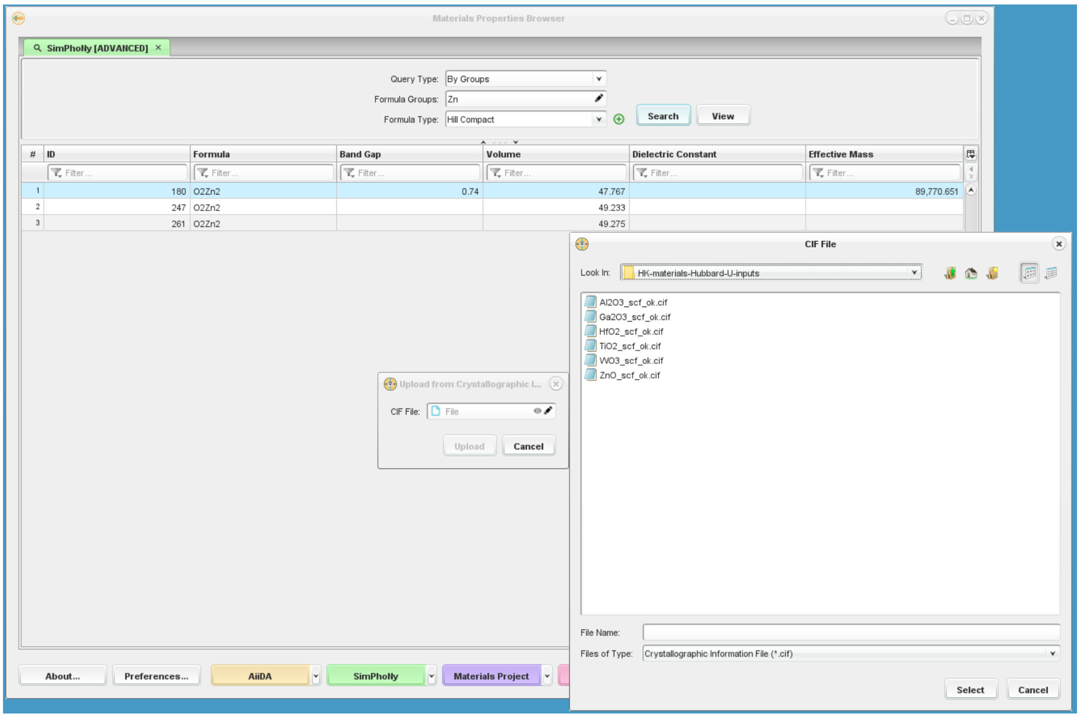

Figure 17. Upload a .CIF structure from file list.

- **Submission and monitoring of a job**
  - real time control of operations and running codes (Figure 18)

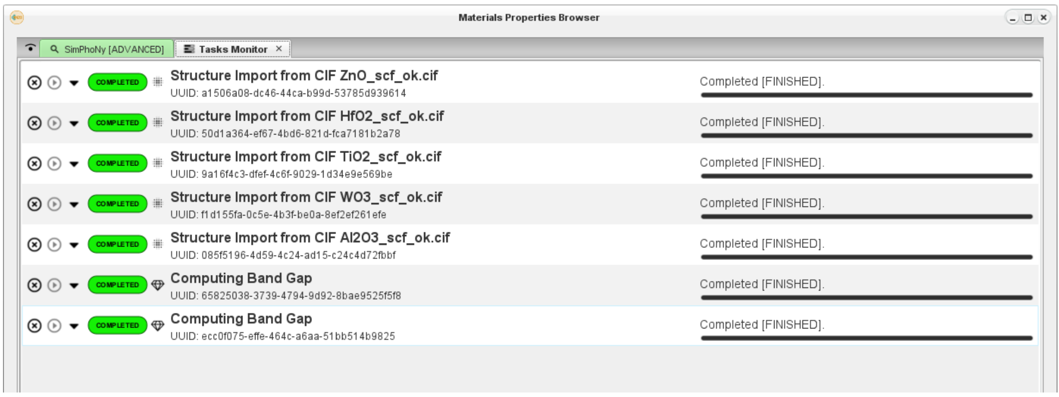

Figure 18. Task Monitor tab.

3. IM2D Database navigation

- Optimade API, connection to other external databases, e.g., Materials Cloud (Figure 19)
- Navigation through the database (Figure 20)

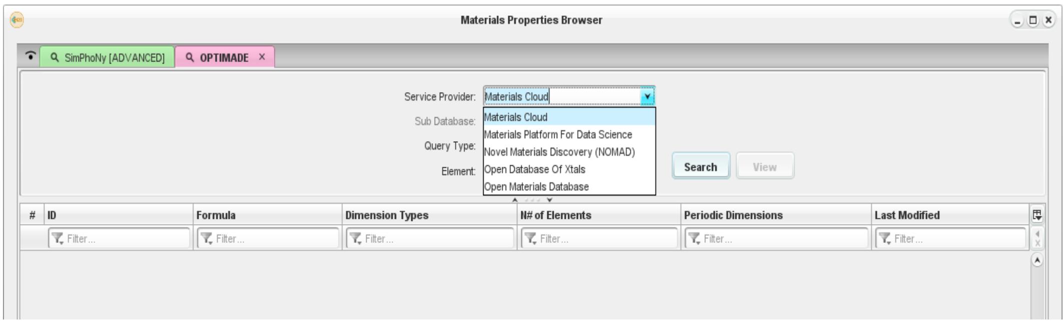

Figure 19. OPTIMADE navigation. Materials Cloud.

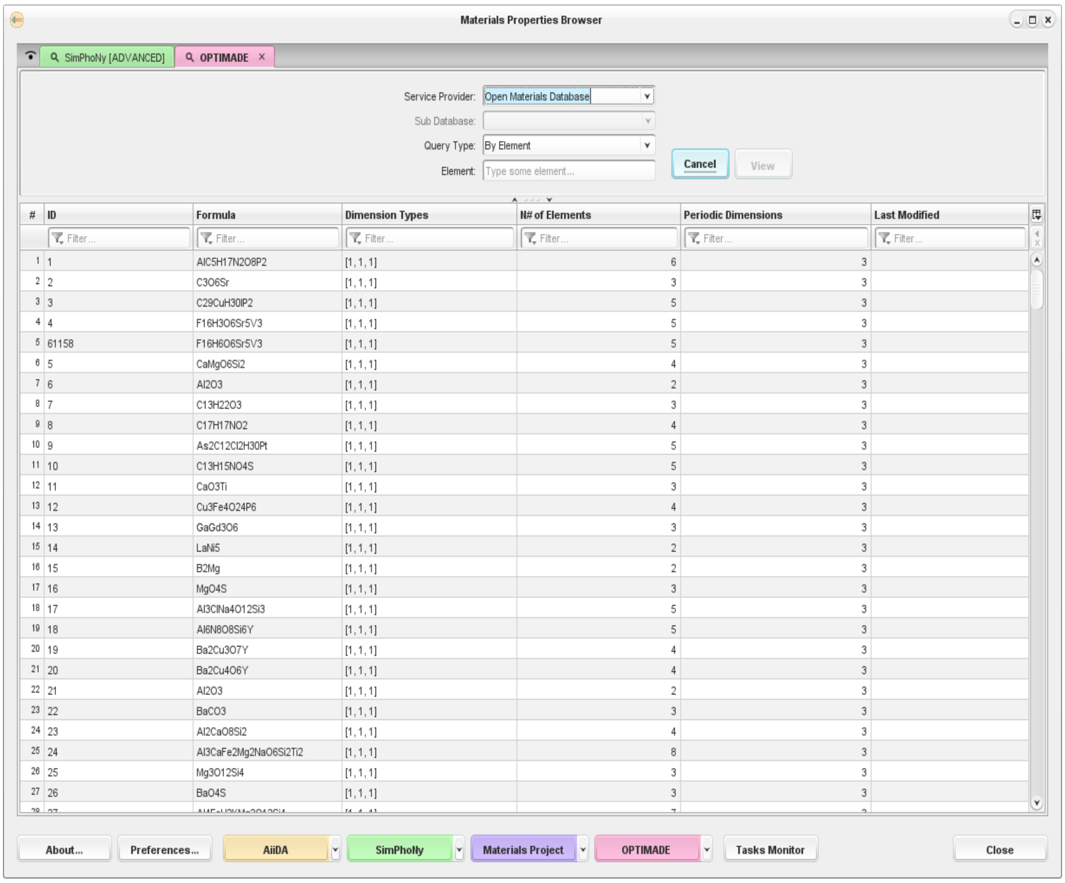

Figure 20. OPTIMADE database Navigation. Open Material Database.

ii. Use case 1: Material-to-Device workflow

In this use case a user can evaluate how the IM2D box is able to accelerate the device design supporting the on-demand simulation of new materials: discover the missing parameters to have a better starting point for the device parameter optimization & design.

As stated in D3.3, the M2D use case deals with:

- how to compute the bandgap for a material using the IM2D box
- how to search the band gap from an external database
- how to use the band gap value retrieved in a Ginestra® MOSFET device simulation

Below the list of main operations to run the use case:

1. **Compute band Gap.** From the IM2D GUI the user is able to launch the AiiDA workflow to perform the calculation of Band Gap by using the Siesta DFT engine (Figure 21).

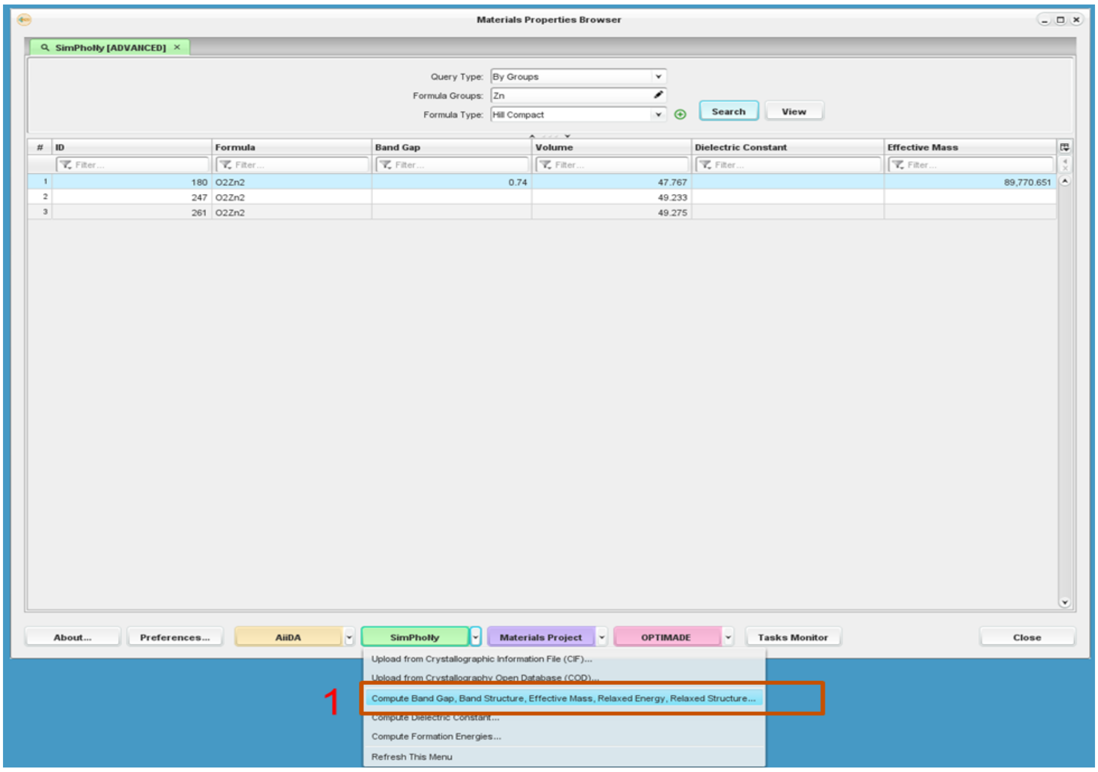

Figure 21. Compute the band gap.

2. **Insert the structure parameters specs.** By Inserting the material information, IM2D generates the input for the Siesta calculation of the band gap simulation.
3. **Consult the "Help" tab**. By consulting the "Help" tab the user can find a list of recommended parameter values without running the computation.
4. **Run the computation** If the preset values are not matching the user desiderata, the code launches the DFT simulation (Figure 22).
5. **Retrieve the bandgap from an external database.** As an alternative to run a new DFT computation, which can be time consuming, IM2D allows users to search directly on the external database to promptly retrieve the information. In this use case we show how to easily find the band gap exploring Materials project (Figure 23).

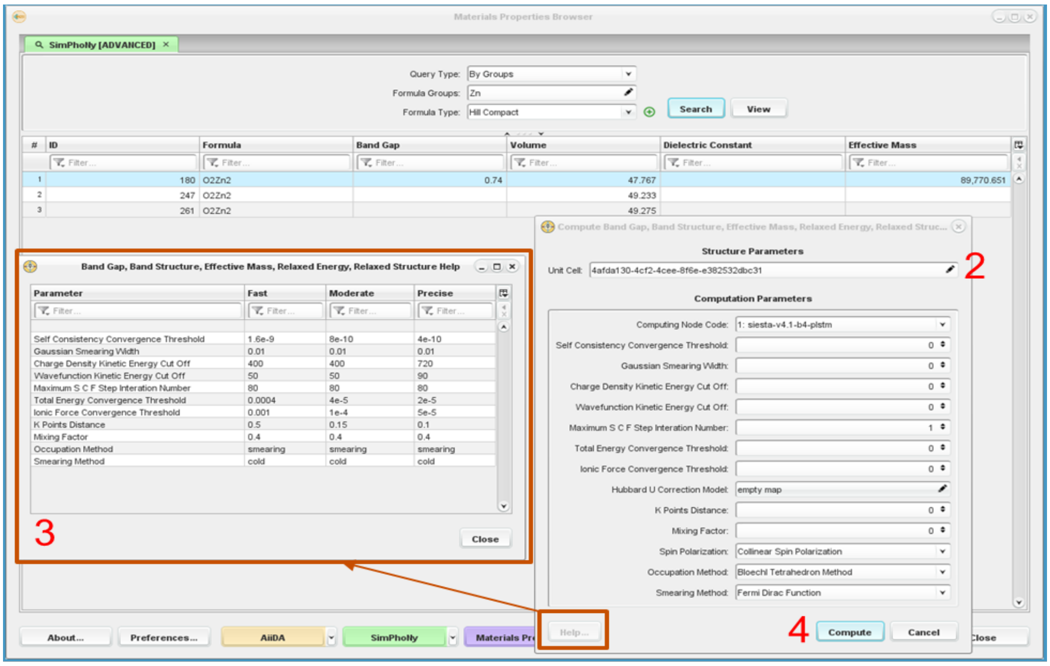

Figure 22. Run the band gap computation

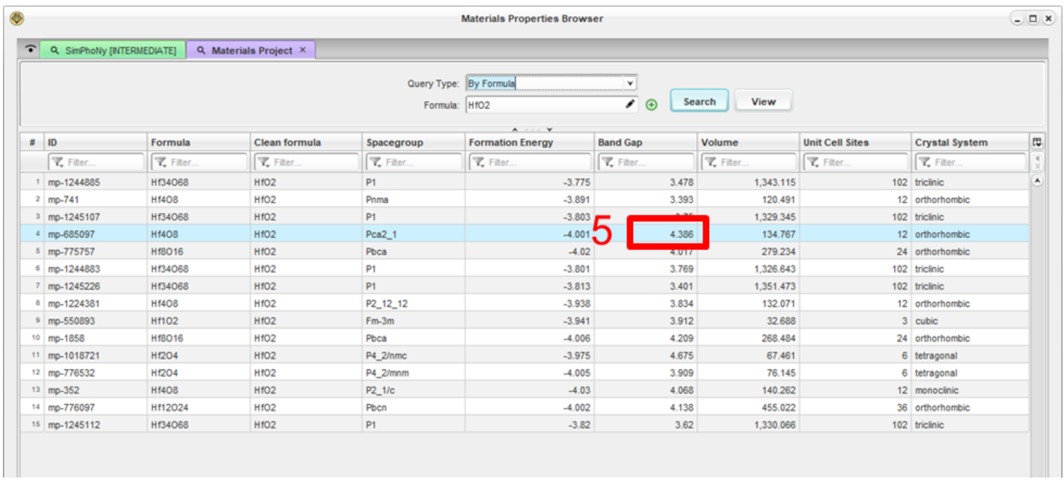

Figure 23. Retrieve parameters from databases.

As extensively described in other Deliverables (D1.4[4], D1.5[5], D1.6[6], D2.5[7], D3.3[8]), one peculiar property of the IM2D box is that - thanks to the semantic interoperability implementation - the compute windows and the help tab adaptively change on the basis of the user's expertise (Figure 24-26).

- **ADVANCED view**

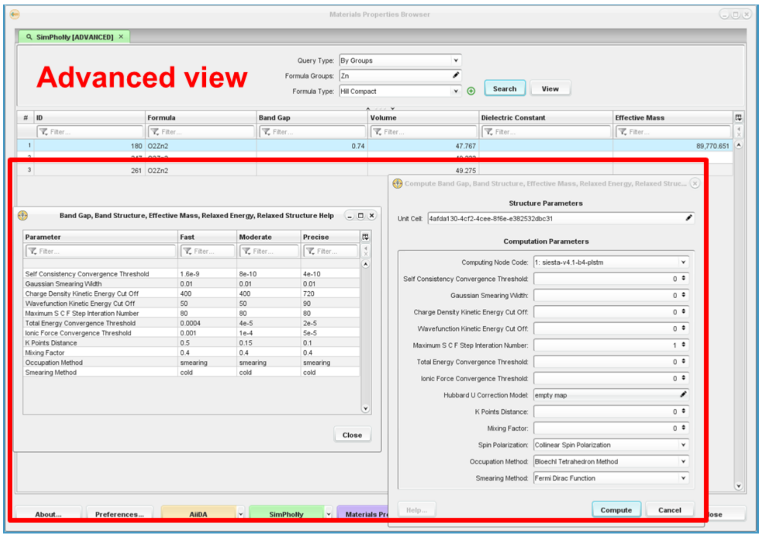

Figure 24. Graphical view setting for ADVANCED users.

- **INTERMEDIATE view**

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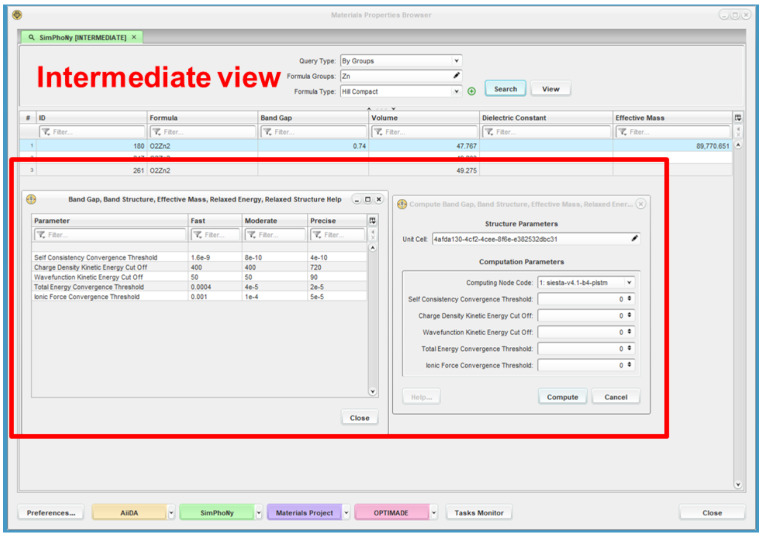


Figure 25. Graphical view setting for INTERMEDIATE users.

- **BASIC view**

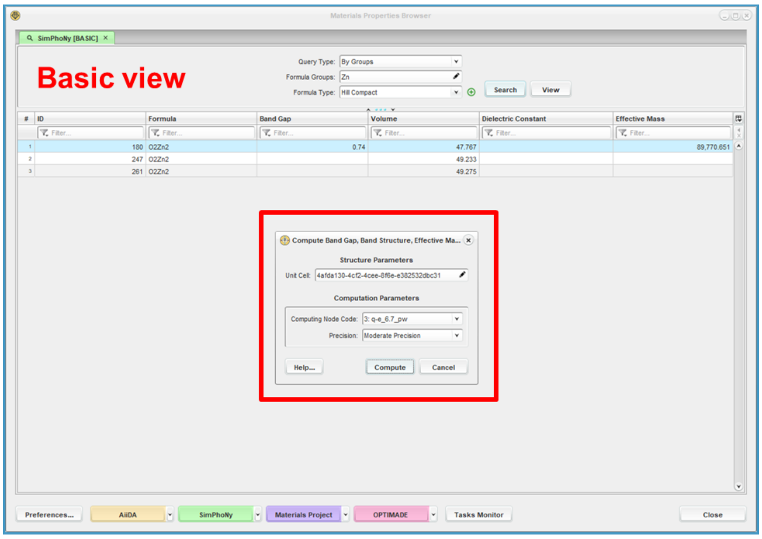


Figure 26. Graphical view setting for BASIC users.

6. **Use the bandgap parameter on a Ginestra® MOSFET device simulation.** The resulting band gap value can be inserted into Ginestra® to run in this case a MOSFET device simulation (Figure 27).

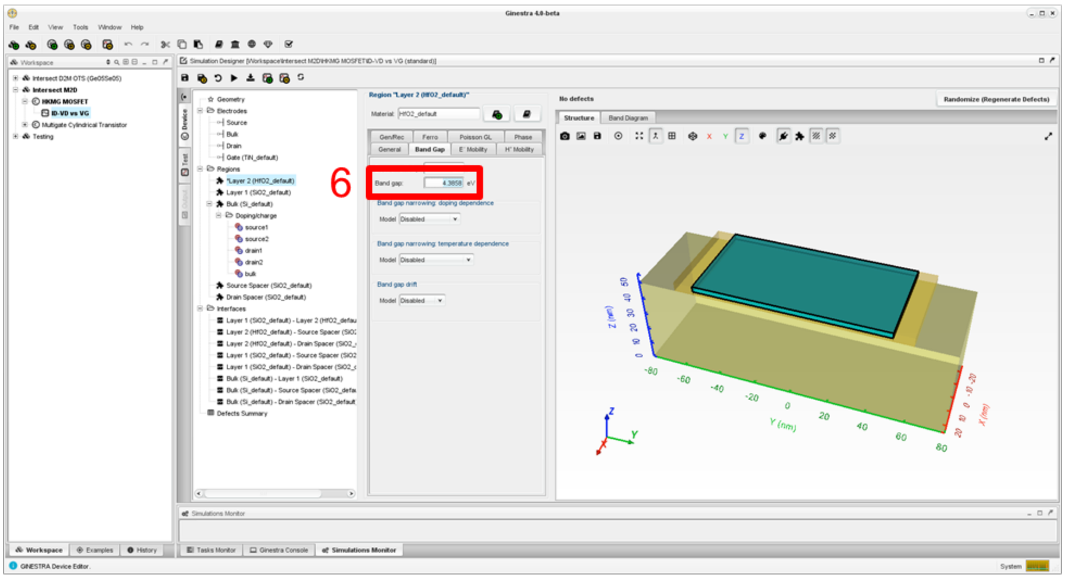


Figure 27. Ginesta® simulation by using band gap data obtained with IM2D

ii. Use case 2: Device-to-Material Workflow

In this use case, a user can evaluate how the IM2D box is able to accelerate the materials characterization, fostering the understanding of the material properties (including atomic defects) from device electrical measurements.

In the following we list the main actions to perform the D2M use case:

1. **Get a set of Device Experimental data**. The starting point is to retrieve a full set of electrical measurements and generate the device model within the Ginestra® software (Figure 28).

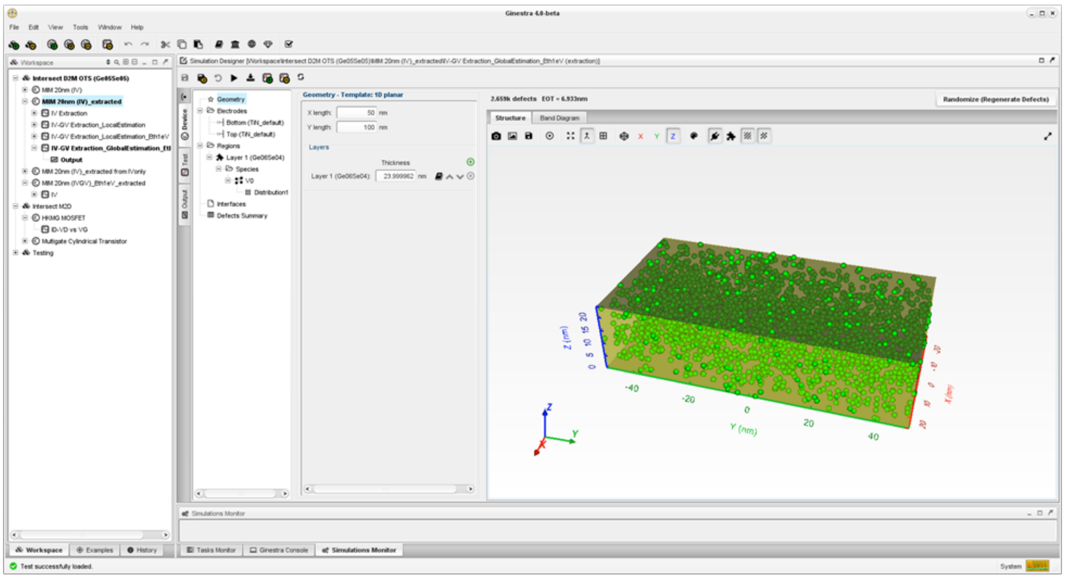


Figure 28. Device model setup, within Ginestra code.

2. Map and Fit the experimental data using Ginestra®

The measured experimental data are loaded into the DDT (Defect Discovery Tool), as a function of the temperature (Figure 29). The material and trap parameters to be extracted (as well as their variation range) are defined in the input file. The selected parameters are automatically varied within the specified intervals until the experimental data are accurately reproduced (Figure 30).

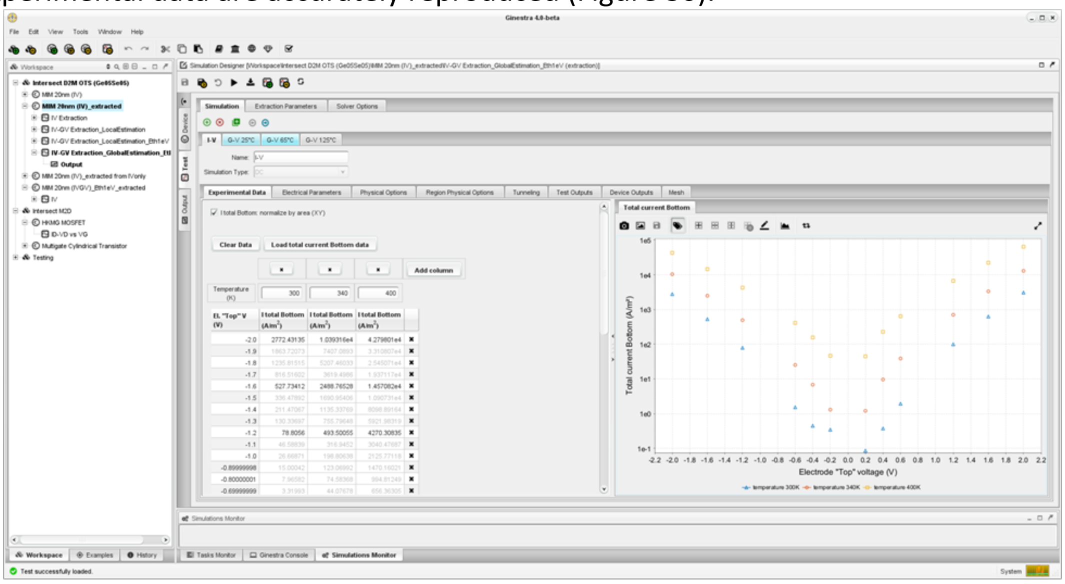


Figure 29. Experimental electrical characteristics are uploaded in the Ginestra® code.

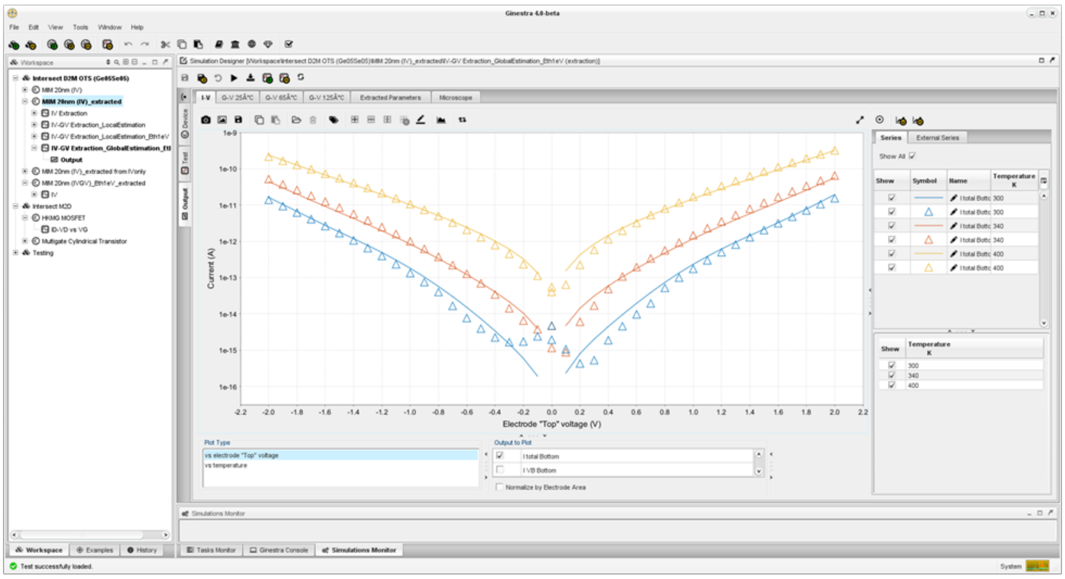


Figure 30. The DDT tool reproduces the experimental data

3. **Use Ginestra® Parameter extraction.** Ginestra®, throughout its DDT tool, is able to extract and predict the materials properties parameters. In this use case we consider the extracted band gap as an example (Figure 31). The list of properties that can obtained is reported in D3.2

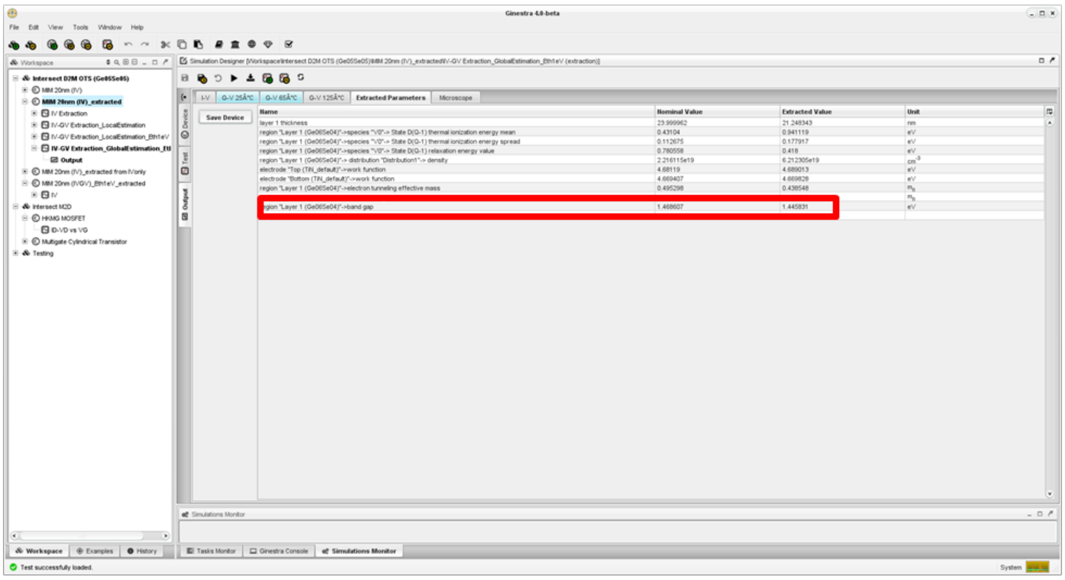


Figure 31. Extraction of material parameters (e.g., band gap) from analysis of electrical characteristics.

4. **Find the material** properties. By using the query filter in IM2D, the user can explore the databases to find the appropriate material composition that best match to the extracted band gap (Figure 32).

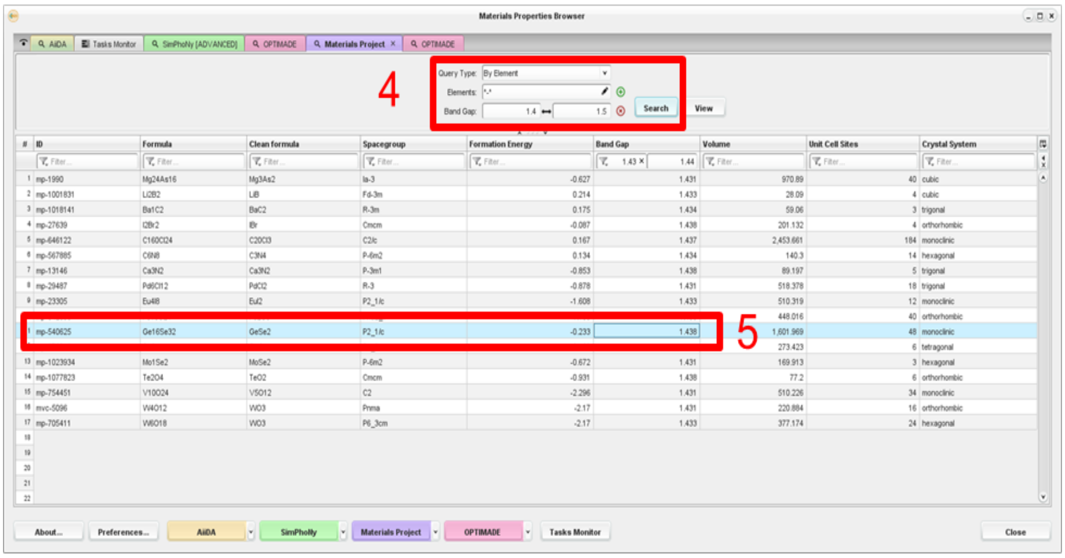


Figure 32. Identification of materials.

5. In this use case, by searching in the Materials Project database we found that the material with band gap 1.438 is the GeSe2. Opening the record (Figure 33), the user can find the data structure and additional material properties to refine its material analysis. If the results do not fit any existing entry of the materials database, the user can launch a new M2D workflow to characterize or discover the material of interest.

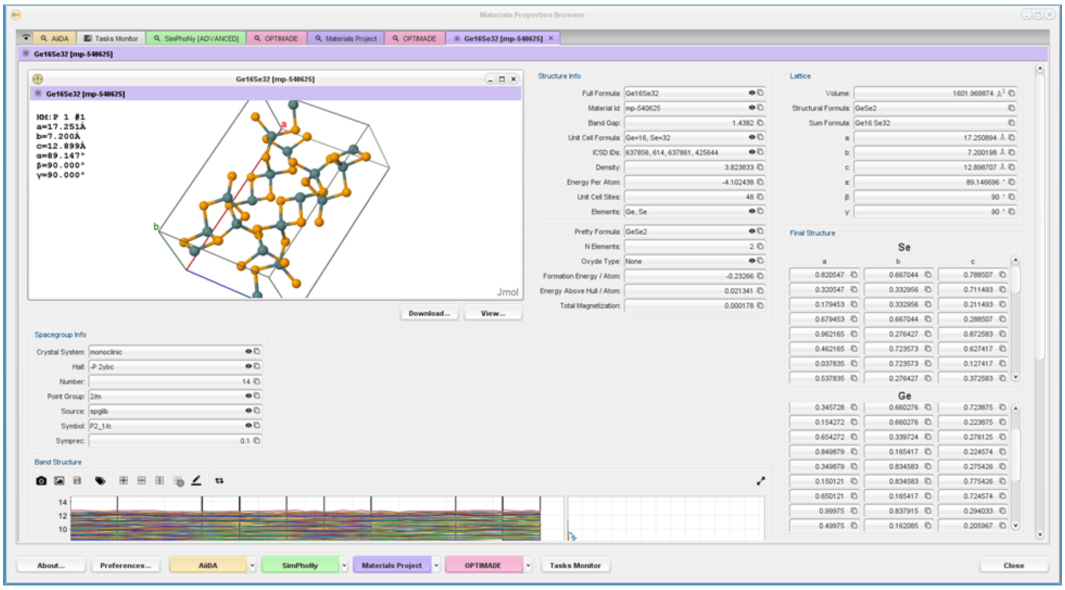


Figure 33. Material Project entry corresponding to the parameters resulting from the DDT analysis.

3.2 Collect Feedback

After the user has performed the above use cases, their feedback has been collected with the survey template described in D3.3. The aim is to collect the user's impression about the functionality, usability, and maintainability of the IM2D box.

Objective:	Collect the user feedback
Input	User type and use case target
Actions	- Target audience will fill the survey. - Collect and sort data - Collect comments
Output	User feedback report

The survey is based on the question collected in Table III:

Table III - User type feedback survey

#	**Question**	**Sub-characteristic**	**Characteristic**
1	All functionality of the software works as expected	Interoperability / Suitability	Functionality
2	The software can exchange information with other software	Interoperability	Functionality
3	The software is easy to operate	Operability	Usability
4	The software does NOT require much effort to operate	Learnability/ Understandability	Usability
5	The software and its results are reliable	Accurateness	Functionality

6	software interface is well organized and attractive	Attractiveness	Usability
7	The software is easy to modify	Extensibility	Maintainability
8	The software works as expected if changes are made	Flexibility	Maintainability
9	Whenever the same operations are performed at any time this software produces the same results	Accurateness	Functionality
10	This software has a very high overall quality		

A score from 0 (Strongly disagree) to 5 (Strongly Agree) has been assigned to each question. Aggregate results for the 55 users have been analyzed on the average of the feedback collected.

#	Question	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know	How can we improve it? Leave your comments/suggestions
1	xxxx	5	4	3	2	1	0	

3.3 Feedback Analysis

The 55 user's feedback surveys have been analyzed by the Management Committee. Following the guideline reported in D3.3, the positive feedback confirmed the IM2D box effectiveness, while negative feedback has been evaluated one by one to identify the root cause/issue and consequently to plan the corrective/improvement actions by using the agile user story approach.

Objective:	Analyze the user feedback and give the input to the development team to improve the platform
Input	User's feedback report
Actions	- Aggregate results to Governing Board - Management Committee analyze the user's comments /suggestions results - Management committee plan corrective/improvement actions creating a set of User stories
Output	User stories Backlog Aggregate results report to Governing Board.

3.3.1 Aggregate results on user survey

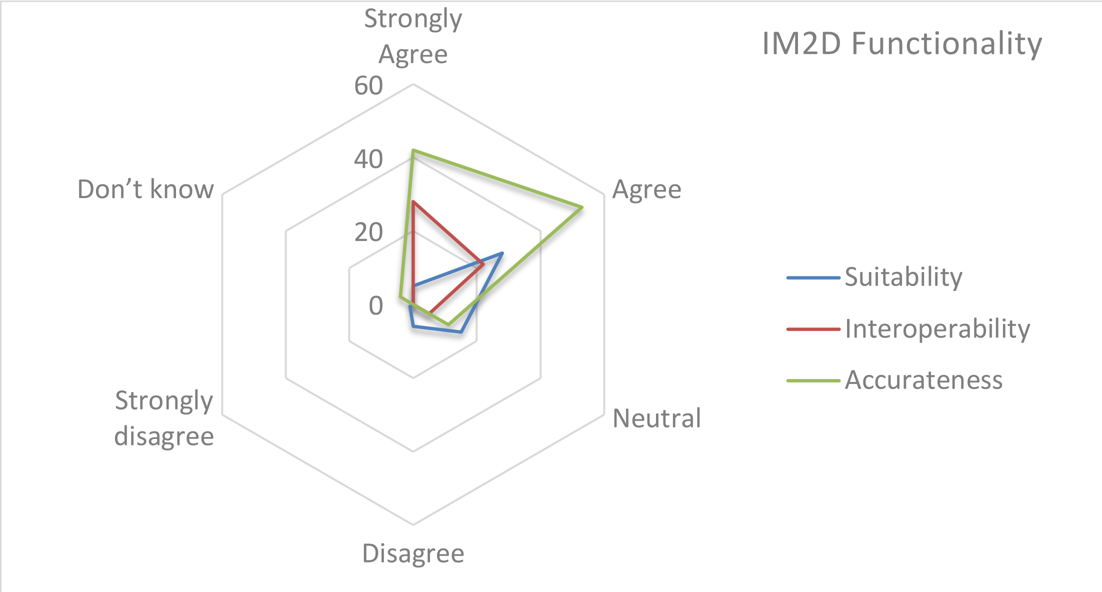
Aggregate results of IM2D User feedback surveys scores have been summarized in Table IV:

Table IV - User survey results

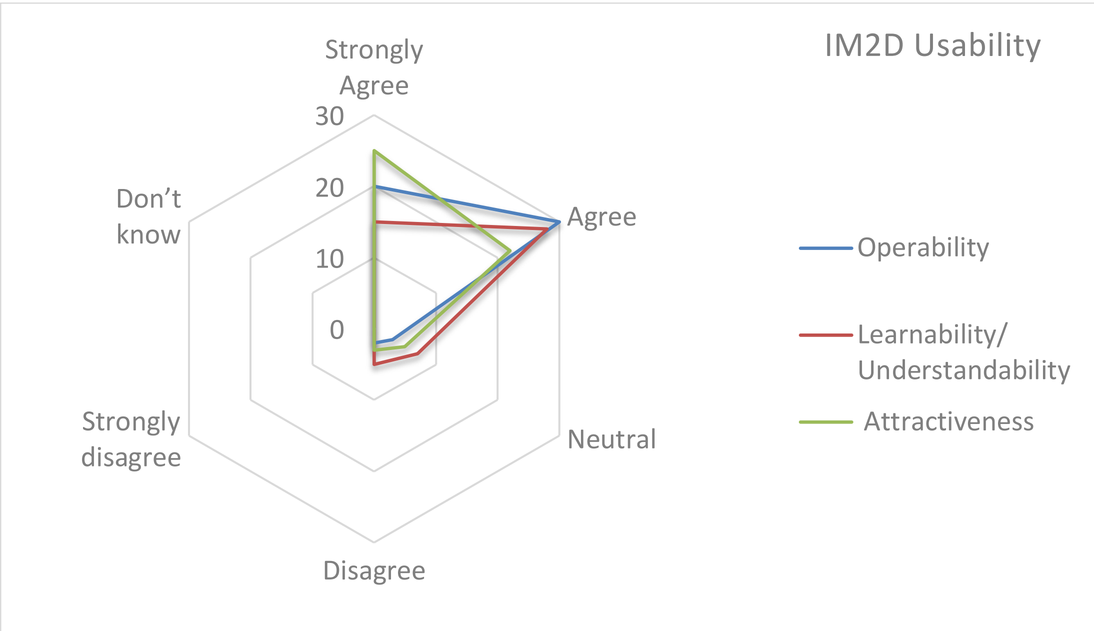
#	Question	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know
1	*All functionality of the software works as expected*	9%	51%	27%	11%	2%	0%
2	*The software can exchange information with other software*	51%	40%	9%	0%	0%	0%
3	*The software is easy to operate*	36%	55%	5%	4%	0%	0%
4	*The software does NOT require much effort to operate*	27%	51%	13%	9%	0%	0%
5	*the software and its results are reliable*	31%	47%	15%	0%	0%	7%
6	*software interface is well organized and attractive*	45%	40%	9%	5%	0%	0%
7	*the software is easy to modify*	15%	40%	18%	9%	0%	18%
8	*the software works as expected if changes are made*	18%	31%	33%	5%	4%	9%
9	*Whenever the same operations are performed at any time this software produces the same results*	45%	49%	5%	0%	0%	0%
10	*this software has a very high overall quality*	42%	47%	11%	0%	0%	0%

Then, surveys results for each FOM characteristics /sub-characteristic have been analyzed:

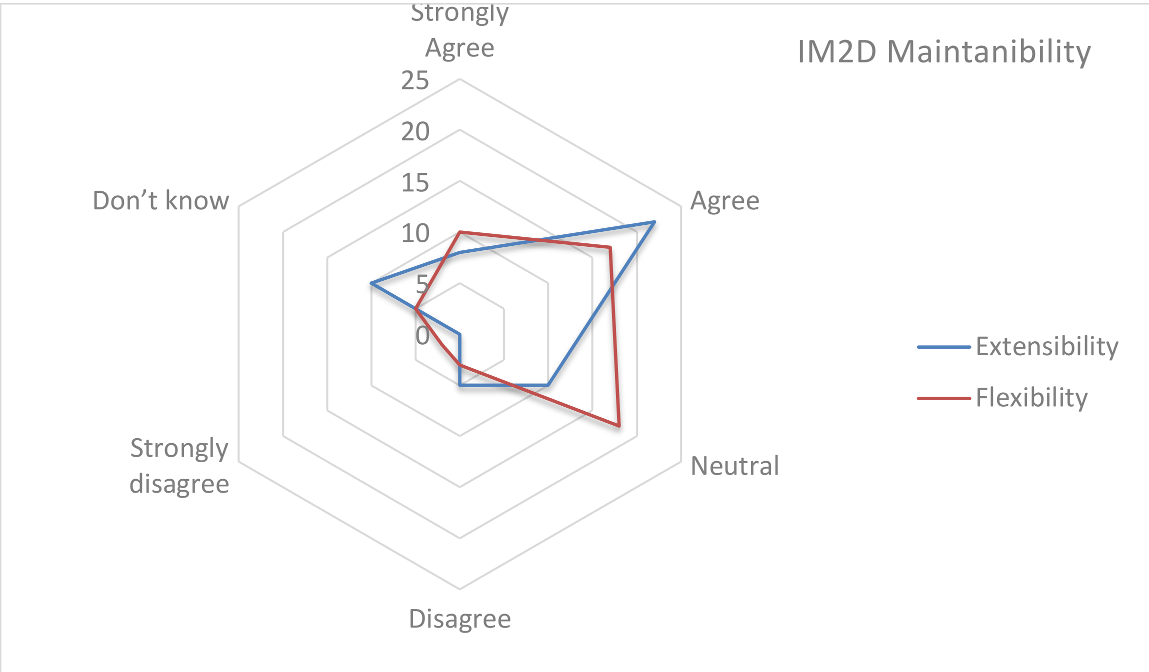
1. **Functionality** sub-characteristics analysis



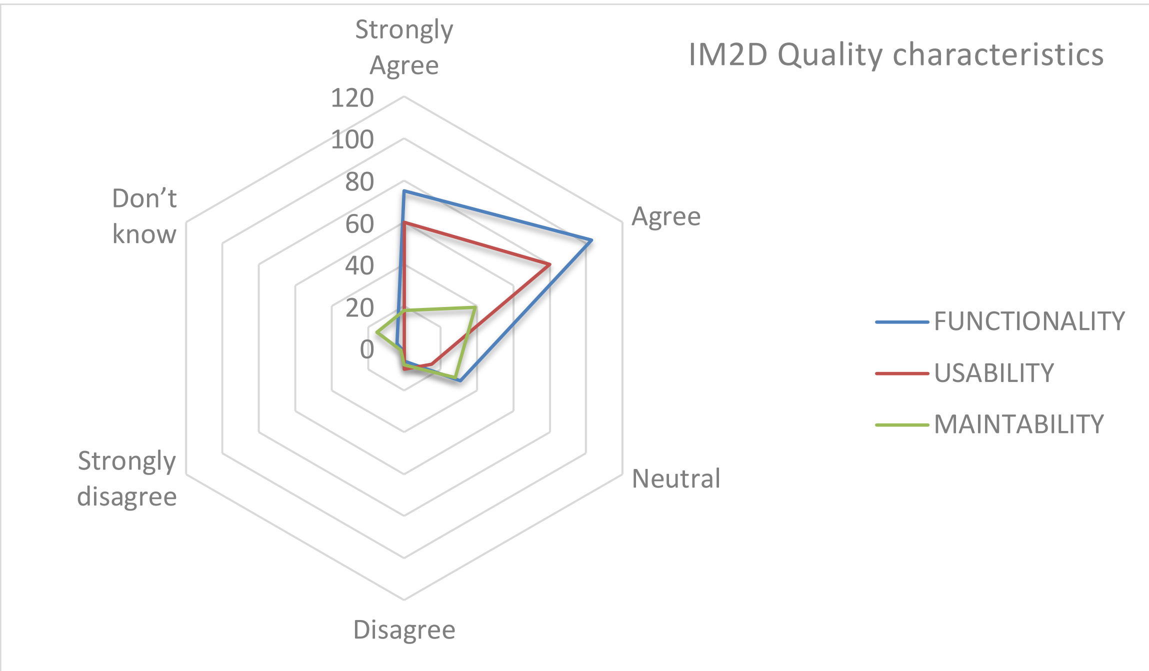
2. Usability sub-characteristics analysis



3. Maintainability sub-characteristics analysis



4. IM2D characteristics analysis



The Feedback analysis indicates that more than 80% of the users are satisfied with the quality FOM functionality, usability, and maintainability of the IM2D box prototype. In particular, users seem to appreciate the graphical interface, the automatic access to databases, and the simple operation mode of IM2D. On the contrary, aspects that should be improved are: the possibility to modify the code and expectation of the existing functionalities, which relies on the knowledge levels of the users (e.g., further enlarging the user story catalog).

3.4 Feedback Implementation

Following an **agile development approach** as mentioned in the D3.3, the IM2D software development team improved the platform based on the User Stories backlog.

Objective:	Improve the IM2D platform development
Input	User stories Backlog
Actions	- Prioritize and implement the corrective/improvement actions. - Deliver the improved IM2D version
Output	New IM2D version

Each team leader will prioritize the user story and implement them accordingly. After the implementation has been done, a new IM2D version will be delivered.

As a general result, 89% of the users are satisfied of overall quality of IM2D box (from Table IV):

#	Question	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know
10	*this software has a very high overall quality*	42%	47%	11%	0%	0%	0%

Considering the results of FOM analysis, to bring the IM2D box from an advanced prototype validated at industrial level to a market-ready product, additional work should be done on the usability and the maintainability (Table V).

Table V - Final analysis of the user survey data

#	FOM	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know
1	*FUNCTIONALITY*	45%	62%	19%	4%	1%	2%
2	*USABILITY*	36%	48%	9%	6%	0%	0%
3	*MAINTANABILITY*	16%	35%	25%	7%	2%	14%

Finally, to evaluate the IM2D development progress across the entire INTERSECT project, we compared the medium score of FOM analysis of the first and second feedback report. As shown in Table VI, in both reports IM2D gets positive feedback (average >=4) for functionality and usability, while further work is needed to improve the maintainability.

Table VI - Comparison between results from first and second report analysis

#	FOM Medium Score	FIRST REPORT	SECOND REPORT
1	*FUNCTIONALITY*	4	4.059
2	*USABILITY*	4.33	4.152
3	*MAINTANIBLITY*	3	3.164

4 Conclusion

This deliverable describes the second user's feedback report to evaluate the IM2D box effectiveness. 55 early adopters from academia (45%) and semiconductor industry (55%), representing user profiles, have been interviewed to evaluate the quality of IM2D box operating in both M2D – Material-to-Device (Use case 1) and D2M – Device-to-Material (Use case 2) way.

The results are promising and indicate positive feedback after the use of IM2D. The general quality indicators improved with respect to the mid-term report (D3.3). The information collected is used to improve the quality of IM2D and make it an appealing tool for industrial users. Other aspects that can be interesting for users (such as documentation, software scalability, installation procedure, GUI navigation, etc.) will be included in the questionnaire list for future surveys.

Acronyms

D2M - Device-To-Material

DDT - Defect Discovery Tool

FOM - Figure of Merit

GUI - Graphical User Interface

IM2D - Interoperable Material-to-Device

M2D - Material-To-Device