D3.3

First report on IM2D box evaluation through user feedback based on the FOMs

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Executive Summary

The present document is the deliverable D3.3 – "First 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" within Work Package 3 – Testing and piloting.

INTERSECT project is developing an industry-ready integrated, standardized, interoperable software platform called Interoperable Materials to Device (IM2D). IM2D will integrate 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 and ontologies, powered by the AiiDA workflow engine, and its data-on-demand capabilities and apps interface.

The scope of Deliverable 3.3 and the Task 3.5 is to evaluate the IM2D box effectiveness during the project enabling the continuous improvement of the platform. This document considers the adoption of the ISO 9126 model for selecting a subset of quality criteria, called Figure of Merit (FOM), appropriate for IM2D user evaluation. A User Survey has been created to collect user feedback. Since IM2D is still in its initial development stage, not all ISO 9126 criteria may be applied yet, and only partial evaluation tests can be actually carried out. Rather, the identification of such self-evaluation criteria from the very beginning of the implementation process allows us to reach the highest quality standards in software production, along the guidelines of Ref. [1] and discussed in deliverable D1.2 (M6).

The data collected here will be analyzed during the review of the INTERSECT analytic user's feedback based on a set of Figures of Merit, which will test also the performances and the quality of the results produced by the IM2D box.

1. Introduction

Quality has to do with feeling comfortable and be satisfied with the user product. At the same time high quality software is an important goal for software developers [1]. INTERSECT focuses on quality assurance of its IM2D platform collecting and analyzing the user feedback following the worldwide standard quality model described on the ISO/IEC 9126 [2]. Software quality can be measured internally (by static measures of the code), or externally (by measuring the behavior of the code when executed). ISO/IEC 9126 categorizes quality from a user perspective as functionality, reliability, usability, efficiency, maintainability, and portability. According to the ISO/IEC 9126 recommendations, INTERSECT chose to evaluate the IM2D box effectiveness considering its **quality in use** (QIU). ISO/IEC 9126 defines 'quality in use' as '*the capability of the software product to enable specified users to achieve specified goals with effectiveness, productivity, safety and satisfaction in a specified context of use*'.

On the basis of the design activity of WP1 and in view of future exploitation (see "First Business plan" D4.3 and "Innovation management plan" D4.5), IM2D platform is realized thinking at well-defined user profiles named ***persona*** (see D1.1 for definition and D1.4 for high level requirements). Thus, the QIU of IM2D is a measure of the performance expectations by selected "persona" that uses this software following the proposed use cases, rather than an analysis of the implemented functionalities. In the initial development stage, we focused on limited sets of *persona* and of physical parameters (See D1.1). The extension to other profiles and the inclusion of new calculated properties, can be straightforwardly done by the implementing specific workflows, univocally planned using MODA schemes (D1.1).

1.1 About this document

The aim of this deliverable is to describe the user's feedback tracking to evaluate the IM2D box effectiveness. The general quality parameters of ISO 9126 model, and the corresponding Figures of Merits will be presented in Section 3. The application of a set of characteristics/sub-characteristics to the INTERSECT problem and their management is reported in Section 4. Section 5 summarizes the first evaluation report on the on-going version of IM2D software, that has been collected from internal (project partner) user's feedback.

2. ISO 9126 Model

The objective in adopting this suite of standards within INTERSECT is to provide a framework for the evaluation of software quality. Among the possible choices in quality assessment, we selected the ISO quality model, as the most complete weaknesses-free model, with respect to other models such as McCall's model or the Boehm model [3]. In addition, ISO/IEC 9126

does not prescribe specific quality requirements for software, but instead describes a quality model, which includes the user view and introduces the concept of **quality in use** that fits with the requirements of Task 3.5.

The ISO/IEC 9126 defines *quality* as '*the totality of characteristics of an entity that bear on its ability to satisfy stated and implied needs*.' The ISO/IEC 9126-1 defines a quality model with six characteristics namely, **functionality**, **reliability**, **usability**, **efficiency**, **maintainability**, and **portability**. The main description of each characteristic is summarized in Table I.

Table I - Characteristics of the ISO 9126-1 quality model

Characteristic	Description
Functionality	The capability of the software to provide functions which meet the stated and implied needs of users under specified conditions of usage (what the software does to meet needs).
Reliability	The capability of the software product to maintain its level of performance under stated conditions for a stated period of time.
Usability	The capability of the software product to be understood, learned, used, and to provide visual appeal, under specified conditions of usage (the effort needed for use).
Efficiency	The capability of the software product to provide desired performance, relative to the amount of resources used, under stated conditions.
Maintainability	The capability of the software product to be modified, which may include corrections, improvements or adaptations of the software to changes in the environment and in the requirements and functional specifications (the effort needed for modification).
Portability	The capability of the software product to be 'transferred' from one environment to another. The environment may include organizational, hardware or software.

None of the quality factors/ characteristics discussed above can be measured directly and must be assessed in terms of objective sub-characteristics. Sub-characteristics corresponding to the six quality characteristics in Table I are reported in Table II.

Table II - Sub characteristics of the ISO 9126-1 quality model

Characteristics	Sub-characteristics	Description
Functionality	Suitability	This is the essential Functionality characteristic and refers to the appropriateness (to specification) of the functions of the software.
	Accurateness	This refers to the correctness of the functions, and the provided results.

	Interoperability	A given software component or system does not typically function in isolation. This sub-characteristic concerns the ability of a software component to interact with other components or systems.
	Compliance	Where appropriate, certain industry (or government) laws and guidelines need to be complied. This sub-characteristic addresses the compliant capability of software.
	Security	This sub-characteristic relates to unauthorized access to the software functions.
Reliability	Maturity	This sub-characteristic concerns frequency of failure of the software.
	Fault tolerance	The ability of software to withstand (and recover) from component, or environmental, failure.
	Recoverability	Ability to bring back a failed system to full operation, including data and network connections.
Usability	Understandability	Determines the ease of understanding of the systems functions, relates to user mental models in Human Computer Interaction methods.
	Learnability	Learning effort for different users, e.g. novice, expert, casual etc.
	Operability	Ability of the software to be easily operated by a given user in a given environment.
Efficiency	Time behavior	Characterizes response times for a given throughput, e.g. transaction rate.
	Resource behavior	Characterizes resources used, e.g. memory, CPU, disk and network usage.
Maintainability	Analyzability	Characterizes the ability to identify the root cause of a failure within the software.
	Changeability	Characterizes the amount of effort to change a system.
	Stability	Characterizes the sensitivity to change of a given system that is the negative impact that may be caused by system changes.
	Testability	Characterizes the effort needed to verify (test) a system change.
Portability	Adaptability	Characterizes the ability of the system to change to new specifications or operating environments.
	Installability	Characterizes the effort required to install the software.

	Conformance	Similar to compliance for functionality, but this characteristic relates to portability. One example would be Open SQL conformance, which relates to portability of database used.
	Replaceability	Characterizes the *plug and play* aspect of software components, that is how easy is it to exchange a given software component within a specified environment.

3. Quality Model in INTERSECT

The purpose of this deliverable is to establish a quality assessment framework in INTERSECT project, starting from the quality criteria proposed in ISO/IEC 9126. This framework would be used to evaluate 'quality in use' of IM2D on the user case and by the user type defined in the D1.1. According to ISO definition, 'Quality in use' is a term denoting the user's view of quality. External properties (such as functionality and usability) will impact on the observed 'quality in use'. Not-all the characteristics listed above can be applied and evaluated until a first stable version of the code is completed. In this first development stage we focus on three characteristics, namely **Functionality**, **Usability, and Maintainability**, and on few of their sub-characteristics as the initial INTERSECT Figures of Merit to perform the quality evaluation of the IM2D platform (see the Table III). Other quality factors could be introduced with the advancement of the software realization.

Table III – Selected Sub-characteristics of the ISO 9126-1 quality model applied to INTERSECT

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 work as expected?' 'Can the platform interact with all the sub systems?'
Usability (external)	Usability is the key aspect for INTERSECT. IM2D will require a	Understandability	'Does the user comprehend how to

	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.	Operability Attractiveness	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, and its data-on-demand capabilities and apps interface. At the same time, the platform should be flexible to include corrections, improvements or adaptations.	**Extensibility** Flexibility	'Can the software be easily modified?' 'Can the software continue functioning if changes are made?'

Among the sub-characteristic mentioned above, interoperability, and extensibility (e.g. integration) are particularly relevant, as they constitute two of the pillars of the entire INTERSECT project.

Notably, technical tests on accuracy and robustness of single codes and workflows are routinely performed. For example, AiiDA reaches a successful rate of more than 91% in determining the electronic ground state (Figure 1), and 81% in determining the atomic and cell relaxation (Figure 2) of any materials. However, these are intended as *internal* tests to optimize the stability and the efficiency of the of the workflows (materials data 'on demand' in this case) and not as user's validation tests or examples. Thus, even though relevant for the improvement of the overall quality improvement of code, these technical tests will not be considered in the evaluation of the 'quality in use' of IM2D discussed in this Deliverable.

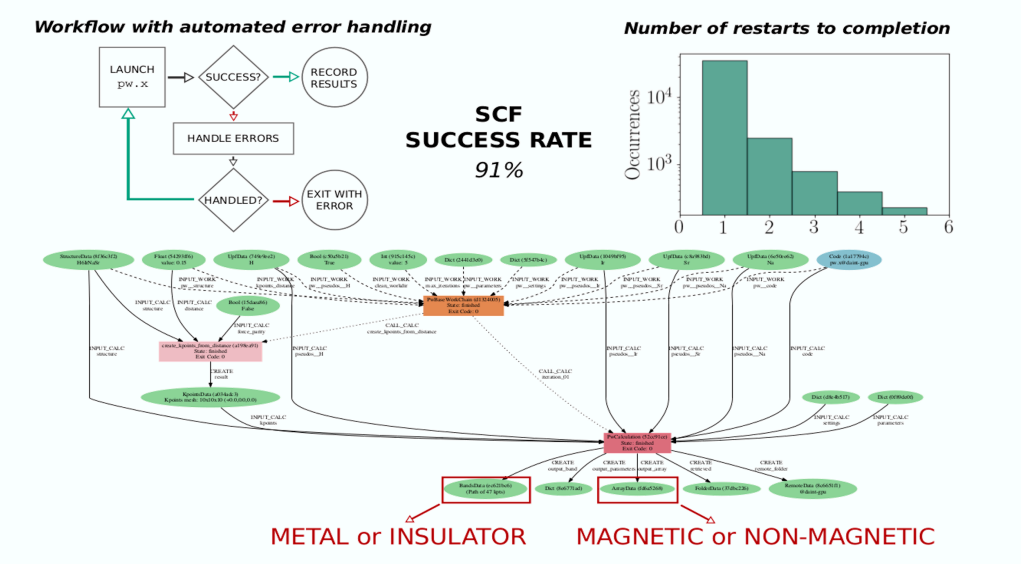

Figure 1: A fully automatic "reconnaissance" calculation using AiiDA-driven Quantum ESPRESSO, to identify the key parameters for the calculation, and the electronic ground-state. Tested over a representative set of 10,000+ materials, it reaches automated SCF in 91% of the case.

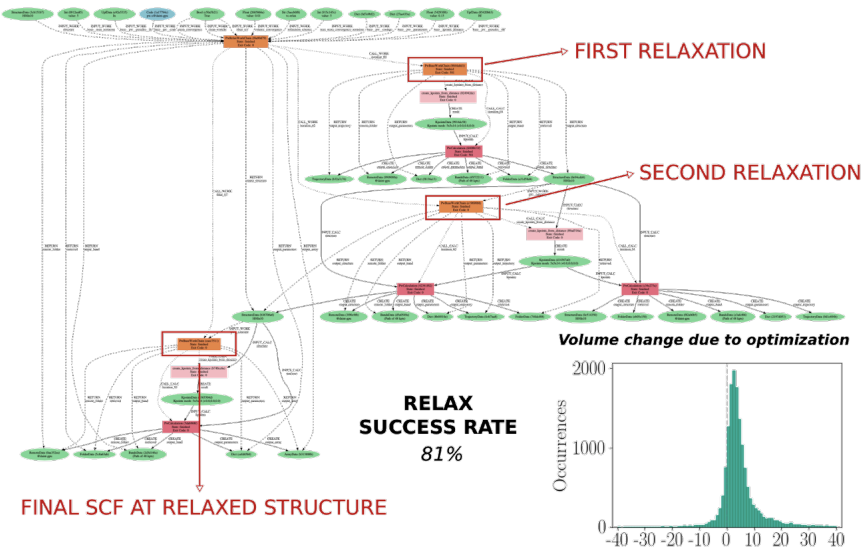

Figure 2: A fully automatic "reconnaissance" calculation using AiiDA-driven Quantum ESPRESSO, to identify the key parameters for the calculation, and the electronic ground-state. Tested over a representative set of 10,000+ materials, it reaches automated relaxation in 81% of the case.

The INTERSECT "quality in use" activity is strongly related to IM2D platform development (WP1.4). Analyzing the user's feedback, the software developer can improve the code and

the user interface to fulfill user requirements, makes it more user friendly and improves the quality standard of the implemented codes.

User negative feedback during the 'quality in use' assessment (e.g. the user is unable to complete a task) is linked to external quality (e.g. suitability or operability). Using an *agile approach*, the feedback will be analyzed by the software development team and turns into corrective actions to fulfill the user requirement. On the other hand, a positive user feedback will validate the IM2D box effectiveness achieving the 'quality in use' for the user type/ case selected.

This approach to software quality is shown in Figure 3.

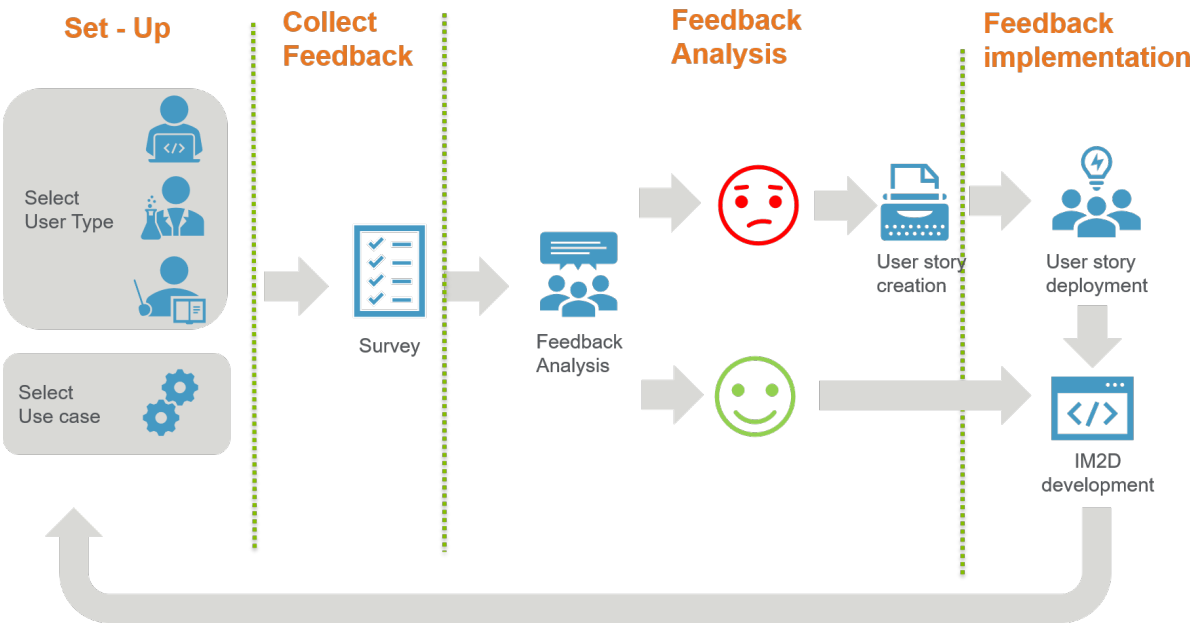

Figure 3 – Quality Assessment Workflow.

3.1 Set-Up

Starting from the use cases and user types identified during the D1.1 a survey session will be organized.

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

The Table IV reports on the type of users (***persona***) to which the quality responsible is going to engage for the quality assessment. The use case will be selected according to the workflow and the list provided in Table 1 of deliverable D.1.1.

Table IV- User type (definitions from deliverable D1.1)

	**Persona #: 1** Process engineer in a company, expert in the optimization/characterization of specific materials but with no experience/knowledge in device modelling (Aa2). This *persona* is the prototypical final user that will use IM2D as a black-simulation box. Participant people from AMAT group in INTERSECT are prototypes of this *persona*.
	**Persona #: 2** Engineer in a company, expert in the optimization/characterization of specific devices but with experience/knowledge in material (electronic/atomistic) models (Ab5). Participant people from FMC/IMEC group in INTERSECT are prototypes of this *persona*.
	**Persona #: 3** Researcher from academy, with background in materials modelling, including electronic models, but with no experience/knowledge in device or circuit optimization (Bc17). Participant researchers from CNR, EPFL, and ICN2 are prototypes of this *persona.*

3.2 Collect Feedback

After the set-up process, the results will be collected from user surveys.

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

During this phase, a user survey will be distributed to the target audience to collect their impression about the functionality, usability and maintainability of the software.

The questionnaire has two sections, the first one defines the test case, the software used, the scope and the expected results from the user perspective. The second section is for the “quality in use” evaluation of the software. The questionnaire is filled anonymously. A survey template for user survey is shown below:

Test-case	
Scope	
SOFTWARE USED	
Expected results	

#	Question	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know	How we can improve it? Leave your comments/suggestions
1	All functionality of the software works as expected							
2	The software can exchange information with other software							
3	The software is easy to operate							
4	The software does NOT require much effort to operate							
5	The software and its results are reliable							
6	Software interface is well organized and attractive							
7	The software is easy to modify							
8	The software works as expected if changes are made							
9	Whenever the same operations are performed at any time, this software produces the same results							
10	This software has a very high overall quality							

A weight for each answer will be assigned (5 for Strongly Agree to 0 Strongly disagree). Aggregate results will be analyzed on the average of the feedback collected.

A score for each answer will be assigned and positive and negative feedback will be sorted out. A User's feedback with more than 3 point will be consider a positive feedback, equal or less than 3 points will be considered as negative feedback. Each negative feedback will be analyzed during the next phase. User's comments will be also collected and linked to the related characteristic to create the user stories during next feedback analysis phase.

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

#	Question	Sub-characteristic	Characteristic
1	All functionalities of the software work 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		

3.3 Feedback Analysis

The User's feedback report created during the previous phase will be analyze by the Management Committee. Positive Feedback will confirm IM2D box effectiveness. Negative feedback will be evaluated one by one to identify the bug/ issues and plan the corrective/improvement actions using the agile user story approach. At the end Aggregate percentage and scores for each

characteristics/sub-characteristic will be reported to the Governing Board to track IM2D user's feedback progression.

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.

In the **agile development approach**, "a User Story tells a short story about the requirements of someone while he or she is using the software product we are building". In our case, IM2D user's comments/suggestions (especially the negative ones) will be analyzed to plan a corrective or improvement action. The advantage of using the user stories is that they precisely focus on what the user needs and wants, without going into the details on how to achieve them. Moreover, INTERSECT involves multiple developer teams in different locations and from different partners: a standard approach like Agile will enforce the communication and the corrective action tracking among the IM2D partner's development team.

As in the D1.1, a well-known and reliable User story template is:

As an [actor], I want [action] so that [achievement]

where:

- The Actor will be associated with the User type category defined in D1.1 for understanding properly the context of the suggestion/comment.
- The Action is what the Actor wants to do.
- The Achievement is what the Actor wants to achieve by performing the Action. That's the Actor's envisioned IM2D result or an IM2D functional technical component that emerges once the Action is completed.

At the end of the analysis, an aggregate results report, with an average score for each characteristic/ sub-characteristic will be reported to the Governing Board to track IM2D user's feedback progression. The improvement of the code towards a better user satisfaction is part of the innovation process (see deliverable D4.5) and is one prerequisite towards the code commercialization (see, e.g., industrial user needs, in deliverable D4.3).

3.4 Feedback Implementation

Starting from the User Stories backlog, the IM2D software development team will improve the platform to fulfill the user requirement.

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

As mentioned, many INTERSECT partners arecinvolved in the IM2D development. Management Committee will assign the right User story to the right team to perform the action. Each team leader will prioritize the user story and implement them accordingly. As all the implementation has been done by the respective development teams, a new IM2D will be delivered.

As a new IM2D release will be available, a new quality session will be setup for continuously improving the platform capabilities and performance.

4. First Evaluation report

For the first evaluation of the IM2D box we focused on a material-to-device (M2D) use case related to feature #2 (Energy band-gap) as listed in Table 1 of the D.1.1.

The current IM2D prototype has been tested by users belonging to the *Persona #2* type (see Table III in Section 4.1). The use case requires to run the Ginestra™ DFT plug-in, developed within the INTERSECT project, to launch an *on-demand* DFT calculation through Quantum ESPRESSO engine, and to obtain the Silicon energy band-gap. Results are imported into Ginestra™ and will be available for subsequent device simulations.

4.1 Use Case Description

The first step of the considered use case is to run the Ginestra™ DFT plug-in from the Ginestra™ GUI (the evolution of Ginestra™ GUI will be the GUI of IM2D platform, see D1.5). This opens the plug-in GUI shown in Figure 4. The highlighted search field [red box in Figure 4(a)] is used to enter the name of the desired material – in this case, Silicon. Once the search is performed by clicking on the *Search* button, the available structures are listed in the dedicated section [see Fig. 4(b)].

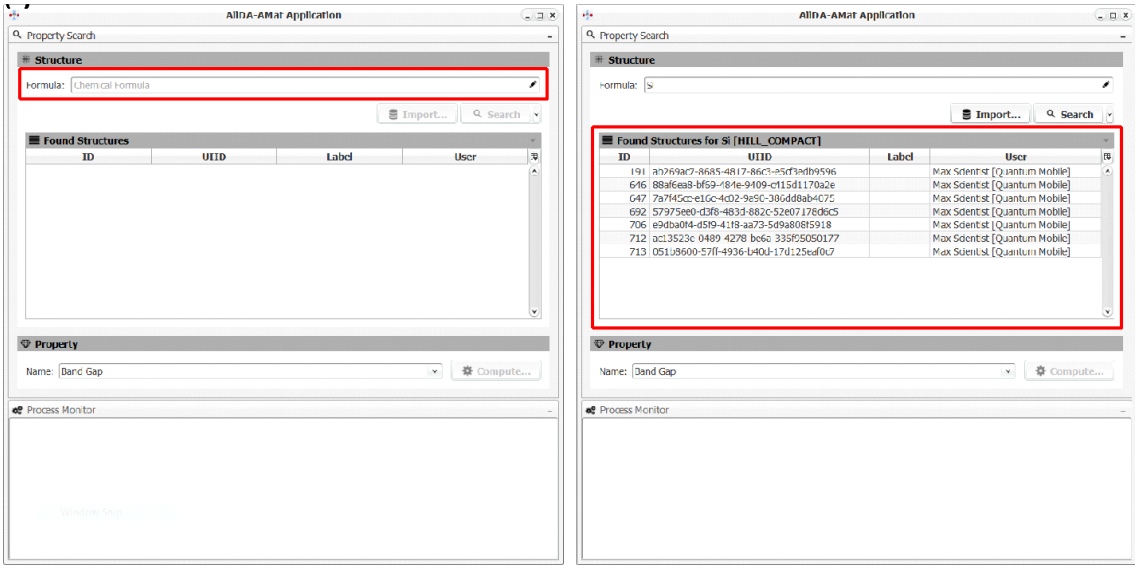

Figure 4 – (a) Graphical user interface of the Ginestra™ DFT plug-in, highlighting the search field to enter the chemical formula of the desired structure. (b) Once the search for the desired structure (Si in this case) is run, the results (available structures) are displayed.

Selecting one of the recovered structures allows to see its attributes, including the existing computed properties, see Figure 5.

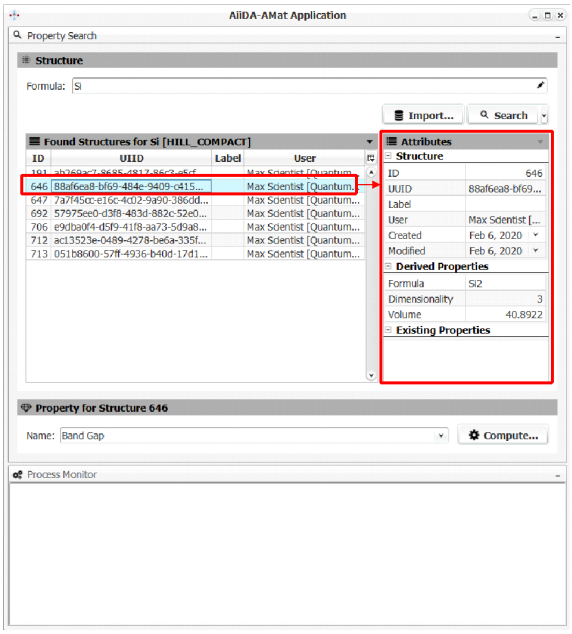

Figure 5 - Graphical user interface of the Ginestra™ DFT plug-in, highlighting the attributes and properties displayed once a structure is selected.

The next step of the test use case is to select a property of the structure to be calculated by means of DFT (band gap in the present case). This requires Ginestra™ to interact with DFT code (QE in this example), by accessing and launching specific AiiDA workflows. Similar M2D path can be done by using SIESTA as DFT code (see D2.1 and D2.2).

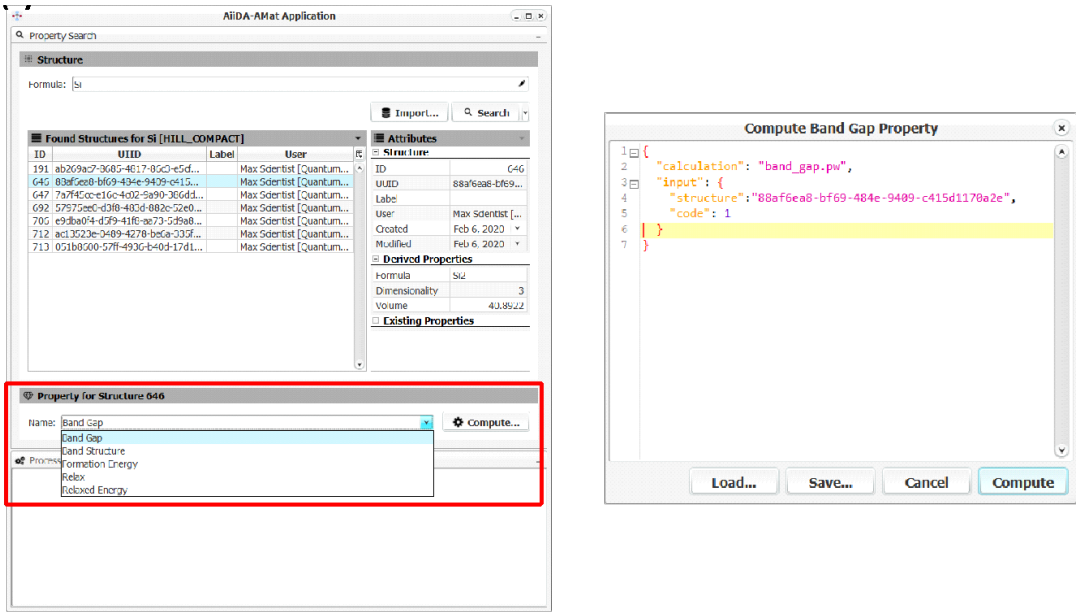

Figure 6 – (a) Graphical user interface of the Ginestra™ DFT plug-in, highlighting the selection of the property to be calculated through the DFT-on-demand approach. (b) example of a json script for the DFT calculation submission.

The desired property is selected from the list of available workflows, Figure 6(a). This opens a dialog window allowing editing a simple *json* script (panel b). The script is automatically generated and permits to run the workflow with default parameters. An advanced user can eventually define and modify the parameters by editing it.

Clicking on the *compute* button submits the energy band-gap calculation to QE through the Aiida workflow. The status of the submitted job can be monitored through the *process monitor* of the Ginestra™ DFT plug-in, see Figure 7. Different labels with different colors are used to indicate the status:

- **CREATED** indicates that the job has correctly been created by AiiDA
- **REFUSED** indicates that the job submission has been refused by AiiDA due to errors in the workflow definition (e.g. misspelled parameters in the *json* script, not existing structure in the AiiDA database, not existing/not connected/turned off computational node, etc.)
- **WAITING** indicates that the job has been submitted and waiting for execution
- **RUNNING** indicates that the job is running
- **FINISHED** indicates that the requested DFT calculation has been successfully completed and the result is available
- **COMMUNICATION** indicates that there is a communication issue with the AiiDA server (e.g. a connection problem) and the monitoring process is not available

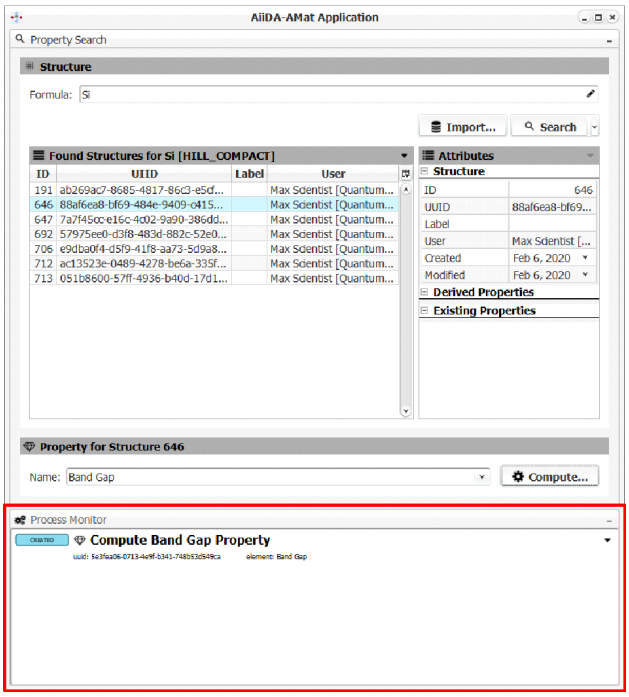

Figure 7 - Graphical user interface of the Ginestra™ DFT plug-in, highlighting the process monitor showing the status of the submitted job(s).

Once the submitted calculation is completed, the status of the job in the *process monitor* changes to **FINISHED**. Right-clicking on the completed job opens a contextual menu allowing to perform several actions. The *Use results* selection allows to copy the result to the clipboard so that they can be imported and used in Ginestra™ (Figure 8).

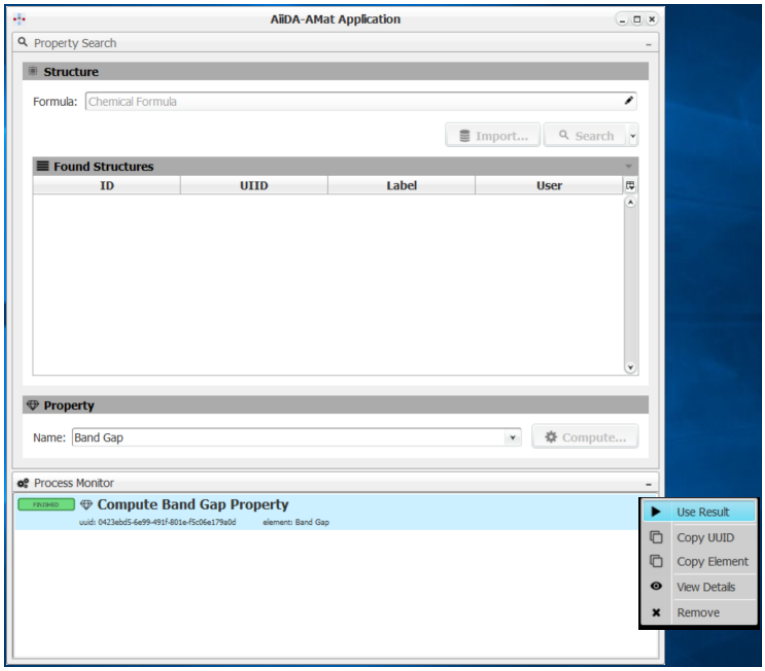

Figure 87 - Graphical user interface of the Ginestra™ DFT plug-in, showing the contextual menu that is opened by right-clicking on a completed job in the process monitor.

4.2 Aggregate results on user survey

The collected results of the user survey based on the results of the use case described in Section 5.1 are summarized in Table V.

Table V- Collected results on the user survey on the selected use case for IM2D testing.

#	Questions	strongly Agree	Agree	Neutral	Disagree	Strongly disagree	Don't know	How we can improve it? Leave your comment or suggestion
1	All functionality of the software works as expected			X				Improve Ginestra™-AiiDA communication as sometimes the plug-in disconnects from the AiiDA server.
2	The software can exchange information with other software		X					
3	The software is easy to operate	X						
4	The software does NOT require much effort to operate		X					
5	The software and its results are reliable		X					
6	Software interface is well organized and attractive		X					
7	The software is easy to modify			X				It was not possible to test this capability
8	the software works as expected if changes			X				It was not possible to test this capability

	are made							
9	Whenever the same operations are performed at any time, this software produces the same results	X						
10	This software has a very high overall quality		X					

5. Conclusions

This deliverable describes the user's feedback tracking to evaluate the IM2D box effectiveness. The quality assessment framework has been illustrated and a list of Figure of Merit has been selected based on the ISO/IEC 9126 standard. A First evaluation report on the developed IM2D has been developed to track internal user's feedback.

ACRONYMS

DFT – Density Functional Theory

FOM - Figure of Merit

GUI - Graphical User Interface

IM2D - Interoperable Material-to-Device

M2D - Material-To-Device

QE – Quantum ESPRESSO

QIU – Quality In Use

SQL - Structured Query Language

References

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