Deliverable D3.6 Second report on IM2D box evaluation



D3.6

Second report on IM2D box evaluation

Valerio Lunardelli, Matteo Bertocchi, Enrico Piccinini, and Arrigo Calzolari

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Authors:	Valerio Lunardelli, Matteo Bertocchi, Enrico Piccinini, and
Additions.	Arrigo Calzolari
	Alligo Calzolali

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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 D3.3². 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 D1.1³. 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 <u>https://intersect-project.eu/wp-content/uploads/2022/04/D3.3.pdf</u>

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.

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

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



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



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

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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).



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 <u>https://materialsproject.org/</u> (Figure 10)
 - OPTIMADE tab: the user can exploit OPTMADE API to query multiple open material database <u>https://www.optimade.org</u> (Figure 11)
 - *Task Monitor tab:* the user can monitor the status of the running jobs.



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(;	₿ <mark>₩</mark> 2D	M	Interope aterial-te		
	APPLIED MATERIALS.	'unec EPFL	Fraunhofer	Ver. 1.1	L.O

Figure 6. IM2D GUI main page.

	tabs below	to get informat	ions about the software and the system.	
About	System	Credits		
			IM2D 1.2	
13	M2	D)	Ver. 1.2.1	
	6190		Release Date: Apr. 13, 2021 COPYRIGHT © 2019-2022 BY APPLIED MATERIALS, INC. www.appliedmaterials.com/indix	
	M2D	standardized exploitation b	able Material-to-Device (IM2D) platform is an Integrated, interoperable software platform conceived for the direct and easy y industrial users to accelerate the development of emerging vices such as FeFET, memristors.	
		-physics and n ific device con	nultiscale approach with focus on novel, complex, "real lifeâ€⊡ figuration.	
			terial and device-driven software, connecting the properties of e electrical behavior of devices.	
	upports two r	nain research	operation modes:	
IIM2D su): optimization of device-design capabilities by understanding and formance starting from the material properties and fabrication	
IIM2D su	predicting process e • Device-to	ffects; - <i>Material</i> (D2M): optimization of material-design capabilities by exploring new ounds, starting from the desired electrical performances of the device.	

Figure 7. IM2D About tab.

www.intersect-project.eu

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					Preferences			
			Ger	-	P Colors Ag	Paging		
Prop	ertes Browser	AUDA	SwPhoRy	Materials Projec				
	Service Base	une la	a /localhost 50	00imi/v4/				
0		-	255, 182, 1		*			
	Displayed Structs							
0	orgunation Paramet							
			Initially Visible					
			Initially Visible					
			Initially Visible					
			Initially Visible					
	Dimensionality Col							
	ectric Constant Col							
	Effective Mass Col							
	lelaxed Energy Col							
			Initially Visible					
			Initially Visible					
			Initially Visible					
	mounted Cal	ant i	comp - nice					
Import	- Expert-		Reset				OK	Carnerd
angeore.	- Cohere		reset					Carrier

Figure 8. AiiDA settings.

				P	references			
			\checkmark	۲	177	ý se		
			General	Forts & Co	Ars Appearanc	Phagins		
1	Properties Drowser A	uDA SimPhe	Hy III	erials Project	OFTIMADE			
	Service Base UPL:	Her Bucaboat	10005840764	,			-	
0	User Expertise				*			
0	Service Color:	ADV/ANCED						
	Computation Parameters:	BASIC INTERMEDIATE						

Figure 9. Symphony settings of persona profiles.

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					Prefere	ences			×	0
				3	P	h	- Sec			
			Gen	eral Fonts	& Colors	Appearanc	e Plugins			
€	Properties Browser Aii	DA S	SimPhoNy	Materials Proj	ject O	PTIMADE				
	Service Base URL:	https://	www.materi	alsproject.org/re	st/v2/					
	API Key:	Rg3Cb0	OuTwUKRC4	julDv						
e	Service Color:	80,	, 1, 255	-		*				
	Pretty Formula Column:	🗸 Initia	ally ∨isible							
	Spacegroup Column:	🗸 Initia	ally ∨isible							
	Formation Energy Column:	🗸 Initia	ally ∨isible							
	E Above Hull Column:	🗌 Initia	ally ∨isible							
	Band Gap Column:	🗸 Initia	ally ∨isible							
	Volume Column:	🗸 Initia	ally ∨isible							
	Unit Cell Sites Column:	🗸 Initia	ally ∨isible							
	Density Column:	🗌 Initia	ally ∨isible							
	Crystal System Column:	🗸 Initia	ally ∨isible							
										1
l	mport Export	Re	eset					(Cancel	

Figure 10. Materials Project settings.

8					Preferer	nces				(
					6		ý			
			Gei	neral Fonts &	Colors	Appearance	Plugins			
• Pr	roperties Browser	AiiDA	SimPhoNy	Materials Project	OPTIN	ADE				
¢ s	Service Base URL:	https://prov	viders.optimade	org/v1/links						
Φ	Service Color:	255, 1,	128		¥					
lana	and Down		Denet					ок	Consel	
Imp	oort Expor	τ	Reset					OK	Cancel	i

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)

			h	Aaterials P	roperties Browser				•	
역 SimPhoNy (ADVAN	iced] ×									
			Query Type:	By Formul	a v					
			Formula	Chemical	Formula					
			Formula Type:	Hill Compa	ct 🗸	Э 🗌	Search View			
					× ×					
# ID		Formula	Band Gap		Volume	Di	electric Constant	Effective Mass		C
🔍 Fiter		🔍 Filter	T Fiter		T Fiter		🗸 Fiter	T Filter		
1	180	02Zn2		0.74	47.3	767			89,770.651	
2	187	Hf4O8			139.5	994				
3		08Ti4			137	.71				
4		O3W			55.					
5		AI406			87.5					
6		02Zn2			49.3					
7		02Zn2			49.1					
8		O2Zn2			49.3					
9		O2Zn2			49.3					
10		03W			56.3					
11		03W			56.2					
12		03W			56.3					
13	354	03W			56.	279				

• Opening a structure data page (Figure 15)





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Figure 14. Materials Data searching using the periodic table.



Figure 15. Open a Data Structure.

$\circ \quad \text{importing of a crystalline structure} \\$

o 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.

SimPhoNy [ADVANCED] ×							
		Query Type: By Gri Formula Groups: Zn	1				
		Formula Type: Hill Co	mpact 👻 🕀	Search View			
ID	Formula	Band Gap	Volume	Dielectric Constant	Effective Mass	13	J .
🐺 Fiter	T Filter	T Fiter	T Filter	T Fiter	Tilter	4	
180	O2Zn2	0.1	47.767	7		89,770.651	
	O2Zn2		49.233	3			
261	O2Zn2		49.275	5			
		Bupboad from Cry CIF Fie: The Uple	stallographic I (x)	sef_ok.cff sef_ok.cff sef_ok.cff sef_ok.cff			
			File Name:				

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

\circ $\;$ Submission and monitoring of a job $\;$

• real time control of operations and running codes (Figure 18)

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C Q. SimPhoNy [ADVANCED] STasks Monitor ×	
⊙	Completed [FINISHED].
⑦ ⑦ ▼ OPELED # Structure Import from CIF Hf02_scf_ok.cif UUID: 50d1a364-ef67-4bd6-821d-fca7181b2a78	Completed [FINISHED].
⑦ ⑦ ▼ ○ ■ Structure Import from CIF TiO2_scf_ok.cif UUID: 9a16f4c3-dfeF-4c6F-9029-1d34e9e569be	Completed [FINISHED].
⑦ ⑦ ▼ ○ ■ Structure Import from CIF W03_scf_ok.cif UUID: f1d155fa-0c5e-4b3fbe0a-8ef2ef261efe	Completed (FINISHED).
⑦ ⑦ ▼ ○ ■ Structure Import from CIF Al2O3_scf_ok.cif UUID: 085/5196-4d59-4c24-ad15-c24c4d72/fbbf	Completed [FINISHED].
 Computing Band Gap UUID: 65825038-3739-4794-9d92-8bae9525f5f8 	Completed (FINISHED).
	Completed [FINISHED].

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)

•)	Mat	erials Properties Browser			*
	Q SimPhoNy [ADVANCED] Q OPTIMA	IDE ×				
		Service Provider: Sub Database: Query Type: Blement:	Materials Cloud Materials Platform For Data Science	Search View		
	# ID Formula	Dimension Types	N# of Elements	Periodic Dimensions	Last Modified	I \$
	T Fiter	🕅 🏹 Filter	T Filter	T Filter	🟹 Filter	4 X
						۲

Figure 19. OPTIMADE navigation. Materials Cloud.



C Q SimPhoNy (ADVANCED	Q OPTIMADE ×					
		Service Provider.	Open Materials Database	Y		
		Sub Database:		Y		
		Query Type:	By Element	Y		
				Cancel View		
		Liement	Type some element			
ŧ ID	Formula	Dimension Types	N# of Elements	Periodic Dimensions	Last Modified	
T Filter	T Filter	Filter	T Filter	T Filter	T Fiter	
1 1	AIC5H17N2O8P2	[1, 1, 1]	v.	6	3	
2 2	C306Sr	[1,1,1]		3	3	
3 3	C29CuH30IP2	[1, 1, 1]		5	3	
4 4	F16H3O6Sr5V3	[1,1,1]		5	3	
5 61158	F16H6O6Sr5V3	[1, 1, 1]		5	3	
6 5	CaMg06Si2	[1,1,1]		4	3	
7 6	AI2O3	[1, 1, 1]		2	3	
8 7	C13H22O3	[1,1,1]		3	3	
9 8	C17H17NO2	[1, 1, 1]		4	3	
10 9	As2C12Cl2H30Pt	[1,1,1]		5	3	
11 10	C13H15NO4S	[1,1,1]		5	3	
12 11	CaO3Ti	[1, 1, 1]		3	3	
13 12	Cu3Fe4O24P6	[1,1,1]		4	3	
14 13	GaGd3O6	[1, 1, 1]		3	3	
15 14	LaNi5	[1, 1, 1]		2	3	
16 15	B2Mg	[1, 1, 1]		2	3	
17 16	MgO4S	[1, 1, 1]		3	3	
18 17	AI3CINa4O12Si3	[1, 1, 1]		5	3	
19 18	AI6N8O8Si6Y	[1, 1, 1]		5	3	
20 19	Ba2Cu307Y	[1, 1, 1]		4	3	
21 20	Ba2Cu4O6Y	[1, 1, 1]		4	3	
2 21	AI2O3	[1, 1, 1]		2	3	
23 22	BaCO3	[1, 1, 1]		3	3	
24 23	Al2CaO8Si2	[1, 1, 1]		4	3	
25 24	Al3CaFe2Mg2NaO6Si2Ti2	[1, 1, 1]		8	3	
26 25	Mg3012Si4	[1, 1, 1]		3	3	
27 26	BaO4S	[1, 1, 1]		3	3	
10 07	AUE-LOVA-DOADEX	11.1.13		-		

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).

				м	aterials P	roperties Browser					G
۹ :	SimPhoNy [ADVANCE	D] × [O									
				Query Type:	By Group	16	¥				
				Formula Groups:			-				
				Formula Type:		•	▼ ⊕	Search	View		
				Pormula Type.	[Hill Comp	act.	• •				
#	ID		Formula	Band Gap		Volume		Dielectric Cons	tant	Effective Mar	88
	📆 Fiter		🕄 Fiter	Titer		Titer		Titer		T. Filter	
1		180	O2Zn2		0.74		47.767				89,770.651
2		247	O2Zn2				49.233				
3		261	O2Zn2				49.275				
	About	ferences	AliDA	SimPholy Upload from Crystalograph	ic Informat		OPTIMADE	• • •	sks Monitor		Close
	About Pre	ferences	Анда	Upload from Crystallograph Upload from Crystallograph	ic Informat	ion File (CIF) tabase (COD)			sks Monitor		Close
	About Pre	ferences	AHDA	Upload from Crystallograph Upload from Crystallograph Compute Band Gap, Band S	ic Informat v Open Da Structure, E	ion File (CIF) tabase (COD)			sks Monitor		Close
	About Pre	ferences	AiDA	Upload from Crystallograph Upload from Crystallograph Compute Band Gap, Band S Compute Dielectric Constar	tic Informat Ty Open Da Structure, B	ion File (CIF) tabase (COD)			sks Monitor		Close
-	About Pre	ferences	Aida	Upload from Crystallograph Upload from Crystallograph Compute Band Gap, Band S	tic Informat Ty Open Da Structure, B	ion File (CIF) tabase (COD)			sks Monitor		Close

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).

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			Query Type:	By Group	ps	*				
			Formula Groups:	Zn		/				
			Formula Type:	Hill Comp	act	× 😁	Search	View		
# ID	Formula	в	and Gap		Volu	¥ me	Dielectric Cons	tant	Effective Mass	
T. Filter	T. Fiter		T. Filter				T Filter	unic	Titter	
	O2Zn2			0.74	1.44.1	47.767			11 · ·	70.651
100	022n2 02Zn2			0.74		49.233			69,	70.651
	02Zn2					49.233				
201	VELNE							Kenting Mana Del	Energy, Relaxed Struc (x)	
arameter	Fast	Modera			2	Unit Cell: 4afda130-4cf2-4		ition Parameters		-
V Filter	Fiter	T Fite	er 🕅 🏹 Filter			Comp	uting Node Code:	1: siesta-v4.1-b4-plstm		
Self Consistency Convergence Threshole	d 1.6e-9	8e-10	4e-10		1	Self Consistency Converg	anna Thrashold	[0 •	
Saussian Smearing Width	0.01	0.01	0.01			Sell consistency converg	jence miesnolu.			
Charge Density Kinetic Energy Cut Off	400	400	720			Gaussian	Smearing Width:		0 •	
Navefunction Kinetic Energy Cut Off	80	80	90			Charge Density Kinetic	Energy Cut Off:		0 0	
Aaximum S C F Step Interation Number	0.0004	4e-5	2e-5						0 0	
		1e-4	5e-5			Wavefunction Kinetic	: Energy Cut Off:		0.	
Total Energy Convergence Threshold onic Force Convergence Threshold	0.001									
otal Energy Convergence Threshold onic Force Convergence Threshold (Points Distance	0.5	0.15	0.1			Maximum S C F Step In	teration Number:		1 •	
Maximum S C F Step Interation Number fotal Energy Convergence Threshold onic Force Convergence Threshold < Points Distance Mixing Factor Decembing Method	0.5	0.15	0.1 0.4							
iotal Energy Convergence Threshold pric Force Convergence Threshold (Points Distance Mixing Factor Decupation Method	0.5	0.15	0.1 0.4			Total Energy Converg	gence Threshold		0 •	
Total Energy Convergence Threshold onic Force Convergence Threshold < Points Distance	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing				gence Threshold			
iotal Energy Convergence Threshold pric Force Convergence Threshold (Points Distance Mixing Factor Decupation Method	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing			Total Energy Converg	gence Threshold: gence Threshold:	empty map	0 •	
Fotal Energy Convergence Threshold onic Force Convergence Threshold K Points Distance Wiking Factor Docupation Method	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing		0	Total Energy Converg Ionic Force Converg Hubbard U	gence Threshold: gence Threshold:	empty map	0 •	
Fotal Energy Convergence Threshold onic Force Convergence Threshold K Points Distance Wiking Factor Docupation Method	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing		2	Total Energy Converg Ionic Force Converg Hubbard U	gence Threshold; gence Threshold; Correction Model;	empty map	0 •	
iotal Energy Convergence Threshold pric Force Convergence Threshold (Points Distance Mixing Factor Decupation Method	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing	Close		Total Energy Converg Ionic Force Converg Hubbard U (K	gence Threshold: gence Threshold: Correction Model: Points Distance: Mixing Factor:	empty map Collinear Spin Polarization	0 • 0 • • • • • • • • • • • • • • • • •	
Fotal Energy Convergence Threshold onic Force Convergence Threshold K Points Distance Wiking Factor Docupation Method	0.5 0.4 smearing	0.15 0.4 smearing	0.1 0.4 g smearing			Total Energy Converg Ionic Force Converg Hubbard U (K	gence Threshold: gence Threshold: Correction Model: Points Distance: Mixing Factor: Spin Polarization:			

Figure 22. Run the band gap computation

•	Q. SimPhoNy [INT	ERMEDIATE]	Q Materials Project ×							
				Query Type:	By Formula	¥				
				Formula:	Hf02	🖌 🔿 🚺 Se	arch View			
					A					
#	ID	Formula	Clean formula	Spacegroup	Formation Energy	Band Gap	Volume	Unit Cell Sites	Crystal System	
	Titer	T, Fiter	Filter	Filter	Titer	T. Filter	Titer	💘 Fiter	Titter	
1	mp-1244885	Hf34068	HfO2	P1	-3.775	3.478	1,343.115	102	triclinic	
2	mp-741	Hf408	Hf02	Pnma	-3.891	3.393	120.491	12	orthorhombic	
з	mp-1245107	Hf34068	Hf02	P1	-3.803		1,329.345	102	triclinic	
4	mp-685097	Hf4O8	Hf02	Pca2_1	-4.001	4.386	134.767	12	orthorhombic	
5	mp-775757	Hf8O16	Hf02	Pbca	-4.02	4.017	279.234	24	orthorhombic	
6	mp-1244883	Hf34068	Hf02	P1	-3.801	3.769	1,326.643	102	triclinic	
7	mp-1245226	Hf34068	Hf02	P1	-3.813	3.401	1,351.473	102	triclinic	
8	mp-1224381	Hf4O8	Hf02	P2_12_12	-3.938	3.834	132.071	12	orthorhombic	
9	mp-550893	Hf102	Hf02	Fm-3m	-3.941	3.912	32.688	3	cubic	
10	mp-1858	Hf8O16	Hf02	Pbca	-4.006	4.209	268.484	24	orthorhombic	
11	mp-1018721	Hf2O4	HfO2	P4_2/nmc	-3.975	4.675	67.461	6	tetragonal	
12	mp-776532	Hf2O4	Hf02	P4_2/mnm	-4.005	3.909	76.145	6	tetragonal	
13	mp-352	Hf4O8	Hf02	P2_1/c	-4.03	4.068	140.262	12	monoclinic	
14	mp-776097	Hf12024	HfO2	Pbcn	-4.002	4.138	455.022	36	orthorhombic	
15	mp-1245112	Hf34068	HfO2	P1	-3.82	3.62	1,330.066	102	triclinic	

Figure 23. Retrieve parameters from databases.

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As extensively described in other Deliverables (D1.4⁴, D1.5⁵, D1.6⁶, D2.5⁷, D3.3⁸), 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

Advanc	ed v	iew	F	Query Type: ormula Groups: Formula Type:	Zn		× * * •	Search	View		
ID	Formula		Band Gag			ÎVel	ame	Dielectric Cons	fant	Effective Mass	
T Fiter	T Filter		T, Filter		-		Fiter	T. Filter	-curic	There	_
			Y, Fiter.					Tr. Fiter			
1 180	02Zn2				0.74		47.767			89,7	0.651
3 043	007-0		-			-	10.000				
261	O2Zn2						49.275		Nortius Mass Delayed	Energy, Relaxed Struc (X)	
Band Gap, Band Structur	, Effective Mass, I	Relaxed Energy	, Relaxed S	tructure Help		×	Unit Celt 4afda130-4cf2-	Structu	are Parameters		
Parameter	Fast		erate	Precise	p	Ę		Computi	ation Parameters		
V Fiter	W, Fit	er	Filter	V. Filter.		4 X	Com	viting Node Code:	1: siesta-v4.1-b4-pistm		
Self Consistency Convergence Thresh	id 1.6e-9	8e-1	0	4e-10							
Saussian Smearing Width	0.01	0.01		0.01			Self Consistency Conver	gence Threshold.	l	0.0	
Charge Density Kinetic Energy Cut Off	400	400		720			Gaussian	n Smearing Width:		0.0	
Mavefunction Kinetic Energy Cut Off	50	50		90						0.0	
faximum S C F Step Interation Number	80	80		80 2e-5			Charge Density Kineti	c Energy Cut Off:	l	0.	
Total Energy Convergence Threshold onic Force Convergence Threshold	0.0004	40-5		2e-5 5e-5			Wavefunction Kineti	c Energy Cut Off:		0 *	
C Points Distance	0.5	0.15		0.1						1.0	
fixing Factor	0.4	0.4		0.4			Maximum S C F Step I	nteration Number:	l	1.	
Occupation Method	smearin	g smea	ring	smearing			Total Energy Conver	gence Threshold:		0 0	
Smearing Method	cold	cold		cold			Ionic Force Conver	gence Threshold		0.0	
							Hubbard U	Correction Model	empty map		
						۰.	,	Points Distance:		0.0	
					-			Mixing Factor:		0.0	
					Close			Spin Polarization:	Collinear Spin Polarizatio	n ¥	
							00	cupation Method:	Bloechi Tetrahedron Met	hod	

Figure 24. Graphical view setting for ADVANCED users.

• INTERMEDIATE view

⁴ <u>https://intersect-project.eu/wp-content/uploads/2022/04/D1.4.pdf</u>

⁵ <u>https://intersect-project.eu/wp-content/uploads/2022/04/D1.5.pdf</u>

⁶ <u>https://intersect-project.eu/wp-content/uploads/2022/04/D1.6.pdf</u>

⁷ <u>https://intersect-project.eu/wp-content/uploads/2022/04/D2.5.pdf</u>

⁸ <u>https://intersect-project.eu/wp-content/uploads/2022/04/D3.3.pdf</u>



Total 1 100 0 1 100 0 201 0 2 201 0 3 201 0 Band Gap, Band Gap, Band Structure, Parameter Image: Total of the structure, the structu	27.2 Effective Mass, Relax Fast	ed Energy, Relaxed		0.74	V, F	Rer	Triter	89,770.651
Band Gap, Band Structure,	27.2 Effective Mass, Relax Fast					10.000		89,770.651
Band Gap, Band Structure,	Effective Mass, Relax		Structure Help	- 0		49.275		
Band Gap, Band Structure,	Effective Mass, Relax		Structure Help	_ 0		49.275		
Parameter	Fast		Structure Help	- 0				
Parameter	Fast							
			Precise	1		Compute Band Gap, Band Structure, Eff		
¥, 1807			T Filter			Structure Param	eters	
	Titer	V Filter	V. Filter			Unit Cell: 4afda130-4cf2-4cee-8f6e-e382532	dbc31 🖌	
	1.6e-9	8e-10	4e-10					
Self Consistency Convergence Threshol Charge Density Kinetic Energy Cut Off	400	400	4e-10 720			Computation Para	meters	
Wavefunction Kinetic Energy Cut Off	50	50	90					
Total Energy Convergence Threshold	0.0004	4e-5	20-5			Computing Node Code:	1: siesta-v4.1-b4-plstm ¥	
Ionic Force Convergence Threshold	0.001	10-4	5e-5				0.0	
chief of de Contreligende Threations		1014				Self Consistency Convergence Threshold:	• •	
						Charge Density Kinetic Energy Cut Off:	0.0	
						Wavefunction Kinetic Energy Cut Off:	0.0	
						Total Energy Convergence Threshold:	0.0	
							0.0	
						Ionic Force Convergence Threshold:	0.	
				v		Help	Compute Cancel	
				lose				

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).

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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).

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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.

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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

		Ginestra 4.8-beta				
(a) (a) (b) (b) (c) (c) (c) (c) (c) (c) (c) (c) (c) (c		9				
Norkspace Q Q D _ D /	Simulation Designer (V	Workspacelintersect D2M OTS (Ge05Se05)IMM 20nm (Iv)_extractedIV-GV Extraction_GlobalEstimation_Bth1eV (extract	on()			(
& Intersect D2M OTS (Ge85Se85)	88514	1 🐻 🐻 S				
O MM 20nm (IV)	(* IV 0-V 25ÅV	C G-V 65Å*C G-V 125Å*C Extracted Parameters Microscope				
MIM 20nm (IV)_extracted Image: Image in the second secon		Name	Nominal Value	Extracted Value	Unit	
	Save Device	laver 1 thickness	23.999962	21 248343	011	
Interview Content State Sta	lô	region "Layer 1 (Ge06Se04)"->species "\0"-> State D(Q-1) thermal ionization energy mean	0.43104	0.941119	eV	
* N-0V Extraction_LocalEstimation_Bh1eV		region "Layer 1 (Ge06Se04)"->species "\0"-> State D(Q-1) thermal ionization energy spread	0.112675	0.177917	eV	
8 DIV-GV Extraction_GlobalEstimation_Et		region "Layer 1 (Ge06Se04)"->species "\0"-> State D(Q-1) relaxation energy value	0.780558	0.418	e∨	
El Output	Tes	region "Layer 1 (Ge005e04)"-> distribution "Distribution1"-> density	2.216115e19	6.212305e19	cm-3	
IMM 20nm (IV)_extracted from I/only		electrode "Top (TIN_default)"->work function	4.68119	4.689013	eV	
B @ MM 20vm (IVGV) EthteV_extracted		electrode "Bottom (TN_default)"->work function	4.669407	4.669828	eV	
* G N	3	region "Layer 1 (Ge06Se04)"->electron tunneling effective mass	0.495298	0.438548	m ₀	
	8	rgion "Layer 1 (Ge06Se04)"->band gap			n,	
A Intersect M2D	ő	igion "Layer 1 (Ge065e04)"->band gap	1.468607	1.445831	eV	
& Testing						
	100					
	Simulations Monitor					_ 0
Worksport & Exerption & History		Orents Contail of Simulations Monitor				- System

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).

			4	Guery Type: By Element Elements: ** Band Gap: 1.4	 ✓ ✓	View				
ID ID	Formula	Clean formula	Spacegroup	Formation Energy	Band Gap	Volume		Unit Cell Sites	Crystal System	
W. Fiter	Triter	Ther	T Filter	Tter	T. 1.43 ×	1,44 🕄 Fiter.		T Filter	T Fiter	
1 mp-1990	Mg24As16	Mg3As2	la-3	-0.6	27	1.431	970.89	40	cubic	
2 mp-1001831	LI282	LB	Fd-3m	0.2	4	1.433	28.09	4	cubic	
3 mp-1018141	Ba1C2	BaC2	R-3m	0.1	15	1.434	59.06	3	trigonal	
4 mp-27639	128r2	Br	Cmcm	-0.0	17	1.438	201.132	4	orthorhombic	
5 mp-646122	C160Cl24	C2003	C2/c	0.1	17	1.437	2,453.661	184	monoclinic	
4 mp-567885	C6N8	C3N4	P-6m2	0.1	14	1.434	140.3	14	hexagonal	
7 mp-13146	Ca3N2	Ca3N2	P-3m1	-0.8	53	1.438	89.197	5	trigonal	
# mp-29487	Pd6Cl12	Pd012	R-3	-0.8	18	1.431	518.378	18	trigonal	
9 mp-23305	Eu418	Eu/2	P2_1/c	-1.6	38	1.433	510.319	12	monoclinic	
							448.016	40	orthorhombic	
1 mp-540625	Ge16Se32	GeSe2	P2_1/c	-0.2	13	1.438	5 1,601.969	48	monoclinic	
							273.423	6	tetragonal	
3 mp-1023934	Mo1Se2	MoSe2	P-6m2	-0.6	12	1.431	169.913	3	hexagonal	
4 mp-1077823	Te2O4	TeO2	Cmcm	-0.9	91	438	77.2	6	orthorhombic	
¹⁵ mp-754451	V10024	V5012	C2	-2.2	6	1.431	510.226	34	monoclinic	
4 mvc-5096	W4012	W03	Prima	-2		1.431	220.884		orthorhombic	
7 mp-705411	V6018	VI03	P6_3cm	-2	7	1.433	377.174	24	hexagonal	

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.

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

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



#	Question	Strongly agree	Agree	Neutral	Disagree	Strongly disagree	Don't know
1	All functionality of the software works as expected	公 9%	☆ 51%	🏡 27%	🛣 11%	公 2%	公 0%
2	The software can exchange information with other software	☆ 51%	🗙 40%	☆ 9%	☆ 0%	☆ 0%	☆ 0%
3	The software is easy to operate	16%	📩 55%	☆ 5%	☆ 4%	公 0%	☆ 0%
4	The software does NOT require much effort to operate	17%	☆ 51%	公 13%	1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	☆ 0%	☆ 0%
5	the software and its results are reliable	11%	☆ 47%	公 15%	☆ 0%	☆ 0%	🛣 7%
6	software interface is well organized and attractive	숨 45%	☆ 40%	☆ 9%	5%	☆ 0%	☆ 0%
7	the software is easy to modify	15%	📩 40%	🏡 18%	숨 9%	☆ 0%	📩 18%
8	the software works as expected if changes are made	18%	11%	☆ 33%	5%	☆ 4%	1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
9	Whenever the same operations are performed at any time this software produces the same results	숨 45%	☆ 49%	公 5%	☆ 0%	公 0%	☆ 0%
10	this software has a very high overall quality	☆ 42%	☆ 47%	公 11%	☆ 0%	☆ 0%	☆ 0%

Table IV - User survey results

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

1. Functionality sub-characteristics analysis

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2. Usability sub-characteristics analysis



3. Maintainability sub-characteristics analysis

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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%	17%	公 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	25%	☆ 62%	☆ 19%	☆ 4%	<u>ہ</u> 1%	☆ 2%
2	USABILITY	26%	☆ 48%	☆ 9%	🛣 6%	☆ 0%	公 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	🗙 З	☆ 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