An experimentally-validated multi-scale materials, process and device modelling & design platform enabling non-expert access to open innovation in the Organic and Large Area Electronics Industry (MUSICODE)

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Deliverable 7.5

Business Plan for market uptake of project innovations

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PP	Restricted to other programme participants (including the Commission Service)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (excluding the Commission Services)	

Deliverable author(s): D. Di Stefano (ANSYS), E. Lidorikis (UoI)

Contributors: all partners

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Consisting of Coordinator:	University of Ioannina (UoI)	Greece
Partners:	Karlsruhe Institute of Technology (KIT)	Germany
	University of Surrey (SURREY)	UK
	Aristotle University of Thessaloniki (AUTh)	Greece
	Czech Technical University in Prague (CVUT)	Czechia
	Fluxim AG (FLUXIM)	Switzerland
	TinniT Technologies GmbH (TINNIT)	Germany
	Granta design LTD (GRANTA)	UK
	Esteco SPA (ESTECO)	Italy
	Organic Electronic Technologies (OET)	Greece
	Apeva SE (APEVA)	Germany
	ANSYS (ANSYS)	UK
	AIXTRON SE (AIXTRON)	Germany

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Contents

Publishable Summary

MUSICODE is an Open Innovation Platform for Materials Modelling in the Organic Electronics Domain, integrating data management, workflow design and execution, software licensing and HPC support, under a single intuitive and user-friendly interface. This integration, enhanced by the ontological data infrastructure created and the multitude of validated models and modelling workflows, offers a competitive advantage to MUSICODE. This deliverable explains the strengths and weaknesses of the platform and the steps the partners will take to make it sustainable and to exploit it commercially after the end of the project.

1. Introduction

MUSICODE is an Open Innovation Platform for Materials Modelling in the Organic Electronics Domain, integrating data management, workflow design and execution, software licensing and HPC support, under a single intuitive and user-friendly interface. For each part(s) of the tools provided, there are other solutions in the market that are competitive to MUSICODE. However, the combination of all the above under a single platform offers a competitive advantage to MUSICODE. This deliverable explains the strengths and weaknesses of the platform and the steps the partners will take to make it sustainable and to exploit it commercially after the end of the project.

1.1 Objectives of WP/Task

This document describes the effort around WP7/T7.2. The objectives of WP7 are:

- Dissemination & Exploitation of results and IPR management, considering the pre-existing know-how and partner's expertise and the provisions of the Consortium Agreement (CA).
- Organization of Training activities, and promotion of know- how transfer to industries and end-users.
- Business Plan for Market Implementation and future commercialization of the project results.
- Data Management Plan.

The objectives of Task 7.2 are the development & finalization of Business Plan including a full Techno-Economic Analysis and Roadmap for market implementation of MUSICODE innovations, which will include the following:

- Definition of exploitable innovations and their Exploitation Plan (e.g. patents, licensing, etc), in compliance to the signed Consortium Agreement (CA), the MUSICODE Grant Agreement and the agreed IPR strategy.
- Identification of the target markets for the project innovations, including geographical, economic sizes, market trends, main competitors and competitive technologies and approaches.
- Establishment of business model, including marketing strategies, the main client categories targeted, commercialization plan, financial projections (sales forecasts, revenues, cost structures, investment needs, funding strategies, relation to alternative funding sources).
- Establishment of a Sustainability Plan to ensure the continuation and growth of the modelling platform to other OLAE nanomaterials, devices, and products, as well as to other materials, devices, and applications.
- Risk Analysis to identify and assess the factors that could affect the market penetration of the results, financial trends, and technological breakthroughs of related technologies.

1.2 Purpose of this Document

This document outlines the status of the Key Exploitable Results achieved in the project, both individually per partner, and cumulatively regarding the Open Innovation Platform. This includes results, stat-of-the-art, competition, etc. A detailed path towards commercialization is also presented, including strengths and weaknesses, risk analysis, forecasts, etc. Finally, avenues and sources to financing and strategy towards creating an expanding base of users is presented.

1.3 Structure of this Document

Section 2 offers a brief market analysis and view on the competition.
Section 3 details the KERs achieved by each partner during MUSICODE and their individual exploitation plans.
Section 4 described the initial actions undertaken by the consortium towards building an exploitation strategy.
Section 5 describes the joint KER which is the platform itself, its relevance to the market, and risk analysis.
Section 6 goes over the platform key components and the initial sustainability plans for them.
Section 7 describes the initial exploitation business plan including steps towards a legal entity, funding strategies, SWOT analysis, market expectations, forecasts.
Section 8 concludes this deliverable.

2. Market analysis

The global electronic market was valued[1] at over 81.5 B$ in 2022 and it is predicted to reach 500 B$ in 2023, with a CAGR of 20%. The market growth is fuelled propelled by various key factors. One major driving force is the increasing emphasis on sustainability and energy efficiency in technology. Another key factor is the increasingly demand for IoT and wearable devices, for which the flexibility, lightweight and the environmental friendliness of OEs device will play a pivotal role. Finally, the organic electronics sector is witnessing expansion into emerging applications such as healthcare and biometrics (expected CAGR of 23%), offering solutions for flexible and biocompatible sensors, smart bandages, implantable devices, drug delivering systems, etc.

2.1 OPV Market

Predictions indicate that worldwide demand for Organic Photovoltaic Cells (OPVs) is expected to grow quickly in the coming years. This growth is mainly due to the widespread need for effective energy solutions and the rising demand for electricity. It is estimated that by 2028, the market value of OPVs will reach approximately 562.9 million euros, showing a steady increase at an annual rate of 13.5%[2].

Figure 2.1: Global OPV market forecast.

OET has identified three key market areas in the EU and globally for OPV technology, focusing on energy solutions for buildings, vehicles, and automotive industries.

Building Construction (Including Glass, Windows, Curtains, etc.): Buildings are a major source of greenhouse gas emissions and energy consumption in the EU. They account for about 36% of emissions and 40% of energy use. The EU has set rules to improve buildings' energy performance, and by 2028, new buildings will need to include solar technologies. OPVs in buildings can be either built into new structures or added to existing ones, making renovations simpler. The BIPV market, including windows and curtains, is growing rapidly. In 2022, it

[1] https://www.gminsights.com/industry-analysis/organic-electronics-market

[2] *[“Global organic photovoltaics (opv) market report, history and forecast 2015-2026, breakdown data by manufacturers, key regions, types and application”, 2020].*

was valued at approximately 12.83 billion euros and is expected to surge to 79.44 billion euros by 2030[3]. The glass BIPV segment alone is anticipated to grow from 2.02 billion euros to 4.67 billion euros during this period[4].

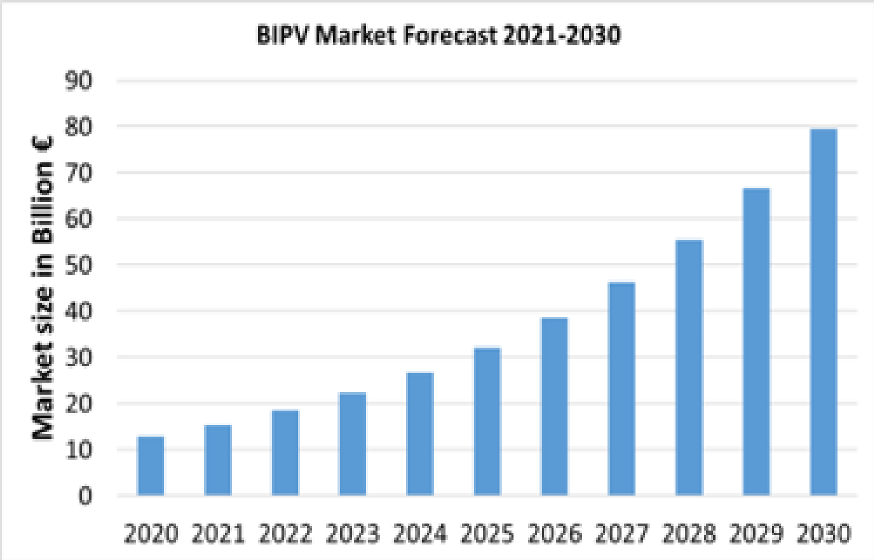

Figure 2.2: Global BIPV market forecast.

Automotive: Vehicles contribute up to 12% of the EU's total CO2 emissions. To reduce this, alternatives to traditional vehicle power are becoming more popular, like electric vehicles (EVs). OPVs can be seamlessly integrated on the EV cars' roof and generate anergy to increase their mileage. The Solar EV market, currently valued at 0.4 billion euros, is projected to grow to 4.85 billion euros by 2030[5].

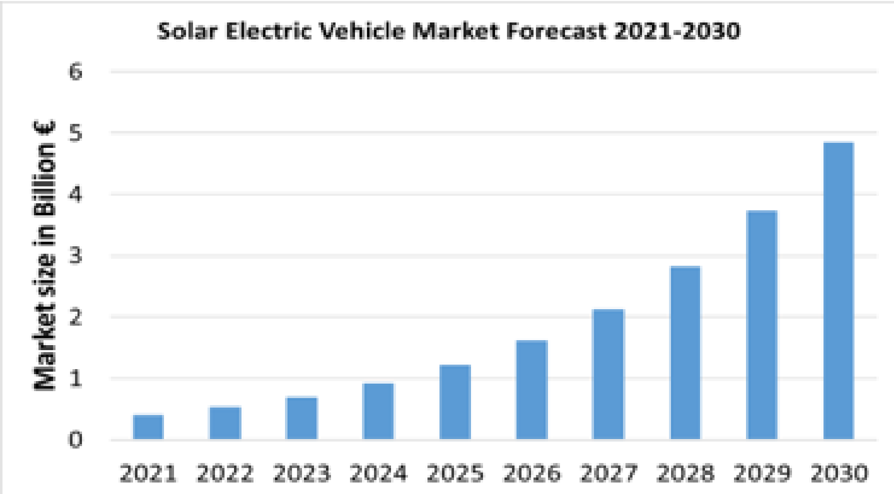

Figure 2.3: Global Solar EV market forecast.

Greenhouse Market: This market includes various types of greenhouses and is valued at 30.6 billion euros, expected to reach 47.1 billion euros by 2025. Using OPVs in greenhouses, and more particularly in Mediterranean Greenhouses which demand a lightweight structure for integration, can significantly save

[3] *MarketsandMarkets, 2022, https://www.reportlinker.com/p05083038*
[4] *E. P. Anil Chaudhary, "Building Integrated Photovoltaics Market by Technology, Application, and End-Use: Global Opportunity Analysis and Indus," Allied Market Research,2021*
[5] *"Solar Vehicle Market 2021 to 2030," Precedence Research, 2021*

energy, grant autonomy, and increase production yield. Mediterranean Greenhouses market is valued at 14.7 billion euros and projected to grow to 22.1 billion euros by 2025.

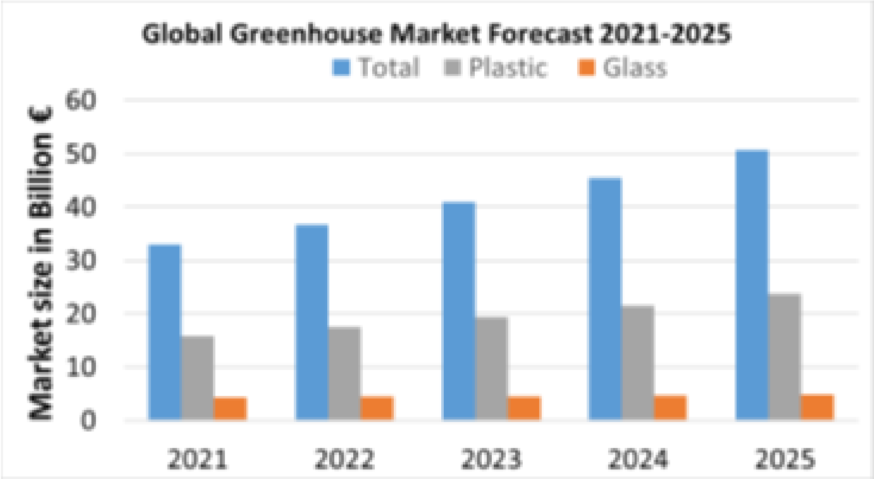

Figure 2.4: Global Greenhouse market forecast.

2.2 OLED Market

OLED panel revenue is set to reach $61 billion in 2026, driven by double-digit CAGR growth in notebook PCs, monitors, and tablets. Smartphones contribute with a 7% CAGR, while OLED Tablets lead the pack with an impressive 27% CAGR, reflecting strong market demand for these devices.

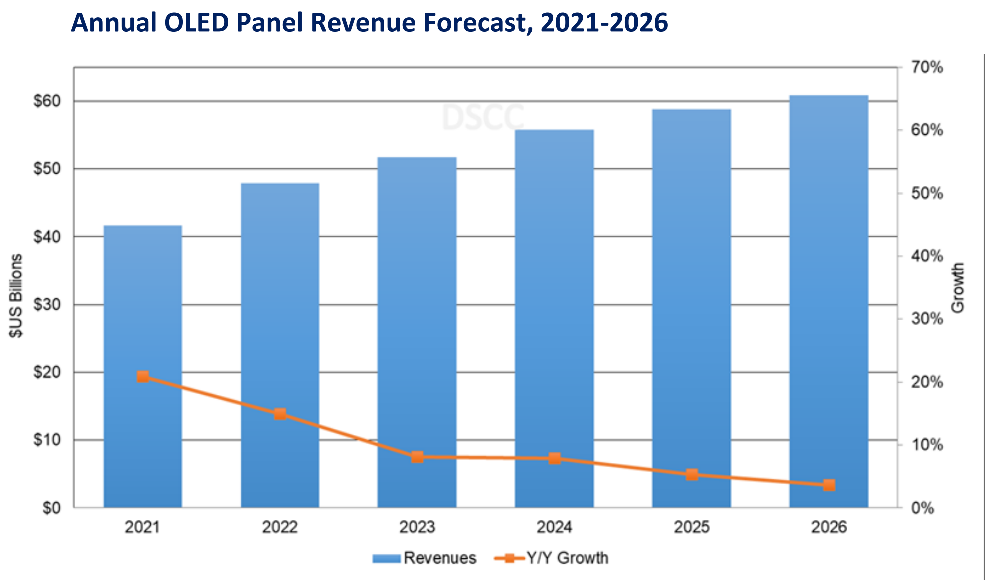

Figure 2.5. Annual OLED Panel Revenue Forecast, 2021-2026

2.3 Modelling Market

Materials informatics is a branch of informatics that aims to improve the development, and discovery of new materials by applying informatics principles to materials science. The global materials informatics market size was valued[6] at 108.6 M$ in 2021 and is expected to reach over 1 B$ by 2030, growing at a CAGR of 26.74%

[6] https://www.precedenceresearch.com/material-informatics-market

between 2022 and 2030. The global Materials Modelling market size has been estimated at 720 M$[7] and it is expected to grow at a CARGR of 8% (estimated from CAE). For a detailed analysis refer to "Materials Modelling Software Market" by Goldbeck Consulting. The materials modelling and informatics market is quite fragmented, especially for low scale modelling. In the following we report on the main organizations with activities around organics electronics modelling and/or offering cloud solution for materials modelling, this is however should not be considered an exhaustive list. All the organizations on the list offer consultancy (services) which is typically a significant, when not the main, part of their revenue and business model.

Biovia (Dassault Systems)

Biovia, part of Dassault Systems, is a scientific software company providing tools and solutions to create new materials and medicines. They provide solvers at virtually any length scale[8] and data/lab management solutions[9], potentially integrated in cloud-based software platform[10].

Schrodinger Inc.

Schrödinger, Inc. is an international scientific software company that specializes in developing computational tools and software for drug discovery and materials science. They offer specific solution for Organic Electronic modelling at low scale (DFT, Molecular Dynamics)[11] and a cloud platform for Materials Modelling[12]

Materials Design Inc.

Materials Design, Inc. creates software products and services for chemical, metallurgical, electronic, polymeric, and materials science research applications. They have some work on organic electronics[13]. They do not seem to offer cloud-based platforms, but desktop solution[14].

Material Square

Materials Square is a cloud-based material simulation web platform service providing physical properties of materials. In addition to the platform, they provide HPC resources as a service[15].

Mat3ra

Mat3ra.com (previously Exabyte.io) is a software company providing a cloud-based software platform[16] which enables materials scientists and engineers in academic and industrial sectors to rapidly adopt and deploy a wide variety of modeling techniques to develop new materials faster. They also offer computational resources.

Citrine Informatics

Citrine Informatics provides an informatics platform that transforms chemicals development through AI embedded in smart data infrastructure. Although focusing on AI they often include physics-based modelling and have example in organic electronics[17].

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[7] https://zenodo.org/records/8101869
[8] https://www.3ds.com/products-services/biovia/products/molecular-modeling-simulation/
[9] https://www.3ds.com/products-services/biovia/products/laboratory-informatics/
[10] https://www.3ds.com/products-services/biovia/products/3dexperience/
[11] https://www.schrodinger.com/science-articles/organic-electronics
[12] https://www.schrodinger.com/products/livedesign/materials
[13] https://www.materialsdesign.com/webinars/recorded/computational-analysis-of-organic-photovoltaics-and-organic-radical-batteries
[14] https://www.materialsdesign.com/medea-software
[15] https://www.materialssquare.com/pricing
[16]
[17] https://citrine.io/panasonic-case-study/

Software for Chemistry & Materials (SCM)

SCM is a software company providing the Amsterdam Modelling Suite, a comprehensive set of modules for computational chemistry and materials science, from quantum mechanics to fluid thermodynamics. They have work in Organic Electronic[18], but do not seem to offer could-based or SaaS solutions.

Microsoft Azure Quantum Elements

Microsoft has recently announced[19] and released (for private preview) Azure Quantum Elements an Azure-based platform to enhance material and chemistry research and development with simulation workflows optimized for scaling on Azure HPC clusters, quantum chemistry solver as a service, AI-accelerated computing, and reasoning using AI[20].

It's clear that there is a healthy thriving market, and so careful due diligence is required to identify strong and weak points relative to competition. However, this also means that there are many opportunities to stand out and offer a competitive alternative. The MUSICODE platform does combine many characteristics that can rarely be found in a single platform, and this makes part of its strength.

[18] https://www.scm.com/applications/organic-electronics/
[19] https://news.microsoft.com/source/features/innovation/azure-quantum-elements-chemistry-materials-science/
[20] https://cloudblogs.microsoft.com/quantum/2023/08/09/accelerating-materials-discovery-with-ai-and-azure-quantum-elements/

3. Individual partner KERs and exploitation plans

3.1 University of Ioannina (UoI)

KER(s) obtained/developed in MUSICODE

The main results obtained by UoI during MUSICODE are:

Advanced, validated models and modelling workflows spanning the electronic-to-mesoscopic scales, applied to materials properties. The properties studied include structural (e.g., glass transition temperature), optical (e.g., dielectric constant), and electrical (e.g., energy levels, mobility), and were very convincingly validated by characterization.

The new software developed in MUSICODE called "PolarShift", performing micro-electrostatics and polarization induction calculations in atomistic systems. This is a versatile semi-analytical tool allowing one to get close to quantum accuracy on large scale molecular systems without having to perform unrealistically large electronic structure calculations. This will be submitted to be published in Computer Physics Communications as an open-source application for use by the modelling community.

All above are tied to the ontological data structures created (data schemata) for organization of complex data, and the use of the HDF5 format to contain, store, and transport the data. Another novel result is the development of model APIs and the model API technology for MUSICODE, applicable and utilizing the MuPIF environment.

Significance and novelty in relation to the state-of-the-art

The model validation achieved in MUSICODE pushes the envelope of the state-of-the-art. The uniqueness of this result is the simultaneous validation of many physical properties, each one on its own being an excellent and publishable result. The complete theoretical and computational construct created in MUSICODE will most certainly make significant impact in the academic community.

The new software includes an extremely versatile input parser accommodating multiple possible input file types, robust routines for the self-consistent calculation of the long-range Coulomb and short-range inductive effects, multispecies input capabilities, parallel processing. Compared to other similar open-source software (e.g., VOTCA, Tinker), PolarShift outstands by being much more user-friendly and intuitive.

Also, the data and workflow technology created, i.e., data structures and schemata, data containers, utilization of MuPIF data services, model APIs, etc, all empowered and facilitated by ontology, is a unique achievement that may have transformative power in the modelling community and may stir significant interest in the industrial community.

Academic/Industrial market analysis and exploitation potential

In the academic world, there are many research groups working on materials modelling using multiscale methods. However, there are notably few that simultaneously address the multitude of physical properties demonstrated here. The publications to be drafted with our results will certainly increase the visibility and recognition of UoI and place it firmly in the forefront of the research activity on organic electronics modelling.

The PolarShift software will enter a small group of relevant software. Given its versatility and the ease in its utilization, there is potential for its wide adoption by the community. This in turn will open opportunities for scholarly recognition, as well as new collaboration agreements.

There is also great opportunity in the science digitalization arena, where the data and model tools (schemata, services, APIs, etc) will play central role. The collaboration with other projects is very important, most notably with OntoTrans on creating fully ontological data schemata and automatic data translators. There is tremendous opportunity in pushing this technology to become the standard in next generation modelling.

Exploitation plan and expected results (1 year and 3 years after project completion)

As an academic group, increased production in publications, citations, and academic recognition are expected because of the MUSICODE activities. Continuing after the end of the project, the application and improvement of the models and workflows will multiply the group's scientific outcome and recognition through papers, citations, and conference presentations.

Regarding the UoI software developed, a good penetration in the open-source scientific solver market is expected. Also, as a follow-up, a second software on kinetic Monte Carlo is in line to be published. This is in its lab phase yet but will be brought into publishable form soon. Both are expected to become standard tools in academic research.

Data tools and models are used within the context of MuPIF and the MUSICODE platform in general. Activities are targeted for continuation after the end of the project within the context of a spin-off company together with other interested partners. This activity is described in more detail in the following sections of this deliverable.

3.2 Karlsruhe Institute of Technology (KIT)

KER(s) obtained/developed in MUSICODE

Extension of phase field model into polymer solutions, using input from both lower (atomistic) and higher (continuum) scales.

Significance and novelty in relation to the state-of-the-art

We are working with different scales such as CFD and MD. The novelty of this work is that the phase field approach has not been applied to the polymer solutions. Therefore, KIT is working in parallel with partners to achieve the new results by linking the scales.

Exploitation plan and expected results (1 year and 3 years after project completion)

So far, KIT is doing the research and has published one paper, and soon the resulting collaboration between TinniT and UOI will lead to the publication of more papers, while the potential for collaboration and publication is high.

3.3 University of Surrey (USUR)

KER(s) obtained/developed in MUSICODE

During the continuation of the MUSICODE project, the Advanced Technology Institute (ATI) at the University of Surrey opened a new research laboratory called "Scaled Printing Laboratory (SPL)". This laboratory is a cutting-edge research facility enabling the fabrication of large-area printed devices such as solar cells, sensors, transistors, batteries and more. It is a research hub for screening and development of novel materials, devices, and concepts. Notably, the laboratory has already been used by external researchers and industrial collaborators.

A detailed description of the printing tools available in the SPL can be found online (see Scaled Printing Laboratory | University of Surrey). So far, the SPL was used for the fabrication of numerous large-scale perovskite devices, as reported in D3.4, and for the deposition of large-scale OPV coatings on perovskite devices.

Significance and novelty in relation to the state-of-the-art

The SPL was set and opened after M12 of the MUSICODE project, and it is a unique research hub – various fabrication tools are accommodated in one laboratory. This allows for the complete fabrication cycle of different large-area devices. Herein, both frontend and backend fabrication activities are possible allowing for the development and manufacturing of a completed product. It must be noted that the fabrication of large-area OE devices and printed electronics was already possible at the ATI, however the technology and process development has had a tremendous improvement since the SPL was opened. Currently, it is possible to fabricate various devices in the SPL, such as large-area solar cells (both OPVs and PSCs), fully bar-coated transistors, sensors for biomedical applications, triboelectric nano-generators, and more. A recent upgrade of the roll-ro-roll coater allows for the slot-die coating of various layers such as perovskite-precursors, metal oxides, organic materials and more, using a continuous deposition process. Currently, the researchers in the SPL working on solar are developing a process for the fabrication of fully slot-die coated solar cells.

Academic/Industrial market analysis and exploitation potential

The interest in perovskite-based solar cells from academia and industry has been very high. This is owed to the similar power conversion efficiencies and operational stabilities of PSC when compared to Si-based SCs but the promise for a reduced levelized cost of electricity for the perovskite technology. The ATI has already gained significant know-how in this solar technology due to the high-impact research, that has been happening in recent years. This is evident from the numerous high-impact publications and industrial collaborations originating from the ATI at the University of Surrey.

Exploitation plan and expected results (1 year and 3 years after project completion)

The University of Surrey plans to continue generating further knowledge in Perovskites. This will lead to the publication of new papers and will attract industrial interest that may lead to future collaborations. If the right circumstances arise, it is also possible that a spinout company will be set up.

3.4 Aristotle University of Thessaloniki (AUTh)

KER(s) obtained/developed in MUSICODE

- Know-how on the fabrication and processing of nanolayers (polymer, organic, inorganic, composite, doped, binary and ternary blends) and devices for Organic Electronic devices, such as Organic Photovoltaics, Organic Light Emitting Diodes, with high efficiency and operational stability as well as Hole-Only devices and Electron-Only devices, by wet, chemical, and vacuum based methods.
- Accurate optical models to model and extract functional parameters (thickness, blend composition, refractive index, band gap, electronic transition energies, Raman shift, etc) from large-sized datasets originating from in-line nano-characterization tools from printing and gas transport processes.
- Optical simulation of multilayer OPV device architectures to achieve specific optical transparency in the infrared-visible-ultraviolet spectrum that can improve the photon absorption, exciton generation and optoelectronic performance of the OE devices.
- Establishment of structure-property relationships for the fabrication of OPV and other OE nanomaterials and device architectures by wet, printing and gas transport processes.

- Further use of the foreground know-how for development and optimization of different devices (e.g. OTFTs, sensors, etc.) as well as to integrate other nanomaterials (e.g. plasmonic nanoparticles, nanowires, graphene, and other types of two-dimensional materials).

Significance and novelty in relation to the state-of-the-art

The foreground knowledge generated by AUTh during the MUSICODE project and in collaboration with the partners, has a significant importance on the field of Organic & Printed Electronics since it will advance our understanding on the structure-property relationships for a large variety of novel nanomaterials and device architectures for OPVs, accelerating their implementation on upscaled processes for the fabrication of large scale OPV modules, as well as other OE devices. In addition, it fully complements our activities on the development of novel OPV materials and devices by solution-based and vaccum processes.

Academic/Industrial market analysis and exploitation potential

The generated technologies from the AUTh work in MUSICODE is expected to accelerate the development of new materials (electron donors, acceptors, dopants, nanoparticles), OE materials and device processing, optimization of the device architectures (binary and ternary configurations) and optimization of the lab to pilot scale processes for the fabrication of OPVs and other OE devices.

Exploitation plan and expected results (1 year and 3 years after project completion)

The plan to exploit the project results, includes the peer-reviewed scientific publications, patents and i-depots, commercial exploitation of the results, provision of licencing of the infrastructure to academic and industrial entities, the development of products based on OPV devices, the establishment of new collaborations with academia and other research and technology centres in new R&D Proposals and Projects, organization and presentations at major international conferences and events, as well as the expansion of our collaborative network and contributions to industrial Networks and Clusters.

3.5 Czech Technical University in Prague (CVUT)

KER(s) obtained/developed in MUSICODE

MuPIF simulation framework is an original open-source platform with component-based design focused on creation and execution of complex simulation workflows composed from independent models and data sources on distributed and high-performance computing resources. It can be utilized in different areas and disciplines, with applications in design, optimization, or maintenance of any product. It can target academic or industrial users, but there is no commercial support now.

Significance and novelty in relation to the state-of-the-art

User-defined, schema-based containers for storing high-volume unstructured data and semantic data access based on auto-generated methods have been implemented providing versatile data types to represent complex data. The platform has been extended to integrate HPC resources for workflow executions. The user experience has been significantly improved by providing an automatic model API generator, web-based platform monitor, and workflow generator supporting complex logic. Platform TR level is TRL 6 (Technology demonstrated in relevant environment).

Academic/Industrial market analysis and exploitation potential

There is an increasing interest in academia/industry in digitalization of (material) design processes. These processes often require multi-physical, multiscale modeling, leading to integration of different tools and data sources into executable workflows. The platform provides a possible solution. There are several other solutions on the market, with specific advantages and disadvantages. The advantages of MuPIF include its open-source nature, high level of abstraction for models and data, HPC integration and TR level 6.

Exploitation plan and expected results (1 year and 3 years after project completion)

Being open source, the platform targets primary academic users and communities. CVUT will continue to exploit the platform in the frame of its own research, future national and international research projects and in education and training as well. The platform will be further developed and maintained in the frame of existing and future research projects, more specifically for Digital twins. Potentially, the CVUT team behind MuPIF can spin-off a company providing commercial support for industrial customers, depending on the interests of potential customers and availability of suitable funding to start a business.

3.6 Fluxim AG (FLUXIM)

KER(s) obtained/developed in MUSICODE

Within MUSICODE, Fluxim has extended the models used within the commercial simulation software tools “Setfos” and “Laoss”. The tools are used by the industrial and academic market working on emerging photovoltaic (PV) technologies, photodetectors, and light-emitting devices. Within the academic market, the number of publications with the tools provides a good indication about the use for the different applications. From this data, we can see that more than 50% of the publications used Fluxim’s tools for PV applications. The activities in MUSICODE are very much in-line with this focus. Therefore, the user cases are highly important for Fluxim to generate realistic application examples, understand the problems of the market and adapt the workflows accordingly. Within the PV field, most publications are dealing with perovskite-based devices. Specifically for this application area, Fluxim has extended the models to consider photon-recycling (PR) and luminescent coupling (LC) in single-junction and tandem devices.

Significance and novelty in relation to the state-of-the-art

PR and LC models have been developed within MUSICODE. Several application examples have been developed with this new model showing the importance of the effect to correctly predict the performance of perovskite-based devices (PV, but also LEDs). While there are some other reports that show the effect of PR on device performance, they work with a different concept that is physically less sound than the approach chosen by Fluxim.

Coupling the model to existing electrical and optical simulations within the commercial version of Setfos has been executed with scripts. To fully exploit the potential, the new models need to be fully integrated within the commercial Setfos version.

Beside this major effort, Fluxim has also worked on coupling model and simulation software (device – module level) which present a new workflow, especially for non-expert users. Furthermore, we have gained further insights into material parameter determination, especially for charge carrier mobility, which helps us in consulting existing and new users of our characterisation tool Paios.

Academic/Industrial market analysis and exploitation potential

The main markets of Fluxim (emerging PV and OLED) are still growing (see data by OET and AIXTRON). Providing enabling R&D tools, both simulation software and characterization equipment, to those markets offers Fluxim a solid business.

Exploitation plan and expected results (1 year and 3 years after project completion)

Fluxim has published some of the own MUSICODE results and is also interested in publishing results to which we have contributed. In this respect, collaborations with USUR on electrode layout and module design is progressing well (existing blog post and science short). Through this diverse dissemination approach, we target the emerging PV field which is growing in academia but also in industry.

3.7 TinniT Technologies GmbH (TINNIT)

TinniT Technologies GmbH engineering solutions is a cutting-edge company at the forefront of engineering, simulation (TinFlow, StarCCM+, other inhouse solvers), and prototyping, fostering a dynamic collaboration with universities and research institutions. Specializing in transformative solutions, TinniT combines innovative engineering expertise with state-of-the-art simulation technologies to propel groundbreaking prototypes into reality. With a core commitment to research-driven excellence, TinniT maintains robust partnerships with leading universities. These collaborations fuel a constant exchange of ideas, enabling the integration of the latest advancements in engineering and simulation into practical applications. TinniT's strength lies in its multidisciplinary approach, leveraging simulation tools to optimize designs, enhance performance, and expedite prototyping processes. At the center of its activities is the CFD solver TinFlow.

Computational Fluid Dynamics (CFD) is a branch of fluid mechanics that utilizes numerical methods and algorithms to simulate and analyze the behavior of fluid flows. A CFD solver is the software component that implements these numerical methods to solve the governing equations of fluid dynamics. TinFlow uses the fundamental equations governing fluid flow. These are the Navier-Stokes equations, which describe the conservation of mass, momentum, and energy. Depending on the nature of the flow (e.g., compressible, or incompressible, laminar, or turbulent), variations of these equations are employed. TinFlow uses as discretization scheme the FVM (Finite Volume Method). It discretizes the domain into control volumes, calculates fluxes across the faces, and conserves quantities within these volumes.

TinniT's simulation services are offered to the industry in the areas of biotechnology, semiconductor technology, environmental technology, and coating technology. Tasks from these areas concern modeling, simulation, and specialized consulting in the context of process optimization and development of new systems. Methods of customized modeling are used and thus represent a service tailored to customer requirements.

KER(s) obtained/developed in MUSICODE

The MUSICODE project represents a further development and digitalization of this method through the cloud-based WorkFlow concept. It appropriately combines information technology approaches with engineering approaches through the formation of digital twins to the automated implementation of simulation studies, which allows a user to do so without in-depth knowledge to carry out complex cross-scale simulations.

Compared to the initial situation before "MUSICODE", TinniT has created the following significant expansions for this new service environment:

- Development of application interfaces (API) for integrating TinFlow into a data management system.
- Extension and parallelization of the TinFlow internal film model for the prediction of evaporation processes in the production of active layers (organic PV).
- Automation of simulation environment through suitable data interfaces operated by the API.
- Abstraction of the modeling environment through the digitalization of workflows in modeling work.
- Code extension for knudson slip conditions needed for the gas process.
- Integration of a comprehensive substance database with direct connection to the TinFlow solver.
- Integration of the Linux cluster at TinniT for parallel Simulations via the workflow.

- Extension of the API for the use of external HPC resources for large calculation models.
- Building a complex data structure based on the ontology (WP1) with the approach of model management via a repository.

Significance and novelty in relation to the state-of-the-art

To date, TinniT has not been able to offer its industrial customers a consistent simulation platform for tailored calculation tasks. The MUSICODE Platform allows TinniT to offer its calculation services to a new level with advanced features. Software providers of larger software packages such as StarCCM+ (Siemens), CFX & Fluent (Ansys) and CFD-ACE+ (ESI), among others, pursue the goal of making the software available via a cloud in addition to classic software sales and installation for customers. This cloud solution, e.g. Simcenter, enables the use of the software in a cloud (with GUI, etc.) and the execution of calculations on HPC systems that are rented from the provider (AWS) or are connected to the cloud via their own calculation infrastructure. Similar approaches are also being pursued by other providers.

The MUSICODE Platform follows a different concept; rather, MUSICODE provides a calculation infrastructure with the potential for expandability to completely different simulation tools or services, which, in contrast to cloud solutions, enable calculation services tailored to customers. This means software packages from different providers can be integrated into the platform. This is currently being demonstrated in MUSICODE using the example of coating technology for organic photovoltaic layers by coupling CFD with the phase field and molecular dynamics. Here, several scales with the corresponding solution approach are mapped in a workflow. For the end user, this means a reduction in the interaction between the individual tools since the communication levels of the tools are already implemented via the corresponding API for data exchange. Furthermore, the input data can be reduced to a minimum, so that complex calculations can be carried out on a tablet in a validated and secure input mode via a web interface. In the European environment, the calculations are carried out at high-performance data centers, whereby the user does not have to worry about the computer resources. No software installations are required on the customer side; access data and the activation of the model in the customer repository is sufficient to run WorkFlow. The simulation of complex processes is broken down to the essentials. The extent of data entry can be expanded or reduced according to customer requirements. E.g. a customer wants to carry out a CFD analysis to determine a characteristic curve for a customer model. For this purpose, only the points of the characteristic curve need to be specified, e.g. variation of the volume flow.

Fig. 3.1 shows the workflow for the MUSICODE gas process. This workflow represents performing multiple simulations at the push of a button. The volume flow varies in the selected range. The result, and this is also compared to the state-of-the-art, is offered to the customer as a PDF report through automated documentation in addition to the defined field sizes. This makes it possible to immediately generate standardized calculations as well as individual calculations as a report. it no longer needs to be documented.

Academic/Industrial market analysis and exploitation potential

Through the MUSICODE platform and the technology developed, TinniT can occupy a niche in the simulation market and to specifically differentiate itself from cloud systems and to offer a combination of engineering and calculation services for customers from plant engineering and production on an individual level.

In addition to industry, TinniT can also offer services in the academic sector for students and teaching staff that can serve the purpose of training. The integration of university services for expansion or coupling with the TinFlow service can be carried out as part of further research projects.

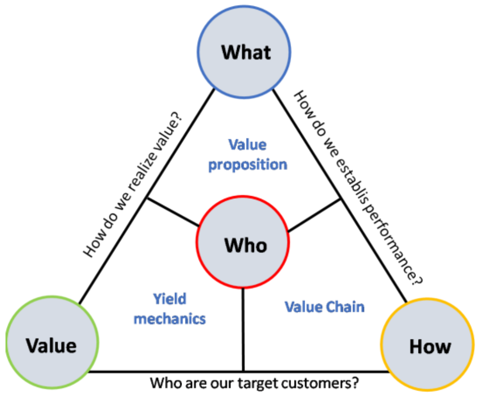

Fig. 3.1: Business model for TinniT services

TinniT has identified the following industries (**who**) for exploiting the results from MUSICODE:

(a) *Biotechnology:* In the field of biotechnology, especially to produce membranes for medical diagnostics and filtration, the physical processes are very similar to the production of organic photovoltaic layers. Here too, coating systems are used that apply a thin liquid layer using the R2R process or to moving belts. The evaporation as well as the heating of the system determines the quality of the porous membrane and thus the capillary liquid transport, which is particularly essential in diagnostic systems. Other membranes, such as in fuel cells or packaging, are analogous in their process; the speed of separation is often crucial.

(b) *Coating machinery producers:* The coating machines as well as the dryers are manufactured by mechanical engineering companies for the manufacturers of specific. materials developed. This development includes the construction and design of the machines for a high level of process reliability for a range of desired products. Machine manufacturers have a great need for advance planning using simulation methods and securing the desired process to save costs, avoid undesirable developments and to be able to analyze in advance the range of application of a machine for the production of special layer structures. Crucial variables such as heat transfer coefficients, energy requirement, evaporation process and final porous material with pore distribution are of great importance. Since the physical processes are extremely complex, they cannot be clearly evaluated without a 3D calculation because the physical quantities are linked to one another (p, T, c, etc.).

(c) Material producers: In addition to the system manufacturers, their customers, the material producers, are of great interest in exploiting the results from MUSICODE. This concerns the fine tuning of the systems through suitable advance calculations of changed process parameters or materials such as the combination of solvents and polymers. In addition to the membrane manufacturers (medical technology), there are other manufacturers of films, org. PV systems, filtration systems etc. interesting for the utilization of the developed methodology. A tool that predicts the process according to changed settings and can provide the system operator with information about the expected quality of the product is very helpful in this context. This also affects system safety (flammable solvents).

Exploitation plan and expected results (1 year and 3 years after project completion, **How, What** and **Value**)

TinniT is currently in discussions with two system manufacturers who develop and build coating machines with subsequent drying units. The dryer system in Thessaloniki, which is used to validate the simulation platform, was manufactured by Coatema, a plant manufacturer. After a confidentiality agreement has been signed, Coatema developers will have access to the MUSICODE platform. Coatema would particularly like to optimize their dryer using the tool developed (WorkFlow concept of the MUSICODE platform). For this purpose, the platform for Coatema will be activated and the dryer model from the repository for simulation studies will be made available for use. A corresponding account should be created for Coatema in the next 2-3 weeks.

Coatema will thus become the first industrial user of the MUSICODE platform. In return, Coatema will provide measurement data from the facility in Thessaloniki for the evaluation. TinniT as well as UOI and CVUT will provide computing resources (HPC, clusters) for temporary use.

In a further step, TinniT will hold a workshop on CFD for coating and drying technology at another company. An essential point here will be the MUSICODE platform, as the company has expressed interest in introducing flow simulation in more detail within the company for its purposes. Finally, TinniT will present the technology developed from MUSICODE to its customers in the membrane production sector and try to recruit a test user for a drying system in the membrane sector. This can certainly be successful. Furthermore, TinniT will specifically present the WorkFlow concept of MUSICODE in the form of lectures, workshops, and publications. It is intended to create a business model concerning the value generation (licensing, project services etc.).

3.8 ANSYS (ANSYS)

KER(s) obtained/developed in MUSICODE

The main KER developed in the project is the REST API for system integration. This is the REST based API developed in WP4 to allow seamless communication between Ansys Granta MI and external tools such as the ESTECO workflow editor and CVUT muPIF simulation platform with the goal to enable managing materials and process modelling simulation results. The API also includes a prototype GUI to facilitate its use.

Additional KERs include:

- Increase knowledge of the OE application area
- Improvements of schema for the traceability of simulation activities
- Improvements of schema for organic electronics
- Demonstrations of the tool

Significance and novelty in relation to the state-of-the-art

As demonstrated in the project. The API is fairly “system” independent, meaning that it could potentially be used to connect Ansys Granta MI to any workflow orchestrator and creation a customers may already use. Not to be at all prescriptive of the tools to use yet to have seamless communication, it is not something that already exists in the market as most commercial solutions are vendor locked-in.

Academic/Industrial market analysis and exploitation potential

The target market will initially be existing customers of Ansys Granta MI which through the API could connect to their existing tools and infrastructure for workflow execution or adopt tools used in the project Ansys sees an increasing interest of their customers on material modelling and related fields and an overall increasing market.

Exploitation plan and expected results (1 year and 3 years after project completion)

As the KER is a TRL5-6, Ansys will need to further develop the API implementation before being able to provide it to customers. There are ongoing discussions to understand the best strategy to bring it forward. The Options considered now are: Ansys internal development, ensure continuation project, or a combination of the two.

3.9 Esteco SPA (ESTECO)

KER(s) obtained/developed in MUSICODE

ESTECO main KER developed in the project is the MUSICODE platform Workflow Editor, more specifically the software module providing the BPMN editing capabilities. To implement the MUSICODE Workflow Editor ESTECO refined the architecture of Cardanit[21] rendering it modular and paving the way for the creation of the ESTECO BPMN editor, a versatile software module for BPMN editing capabilities. The MUSICODE Workflow Editor, developed in WP4, uses the ESTECO BPMN editor, specifically customized for the design of OLAE simulation workflows. The Workflow Editor also includes a verification module and an export module designed to generate MuPIF Python code from BPMN models. While the export module was developed exclusively for the project, the verification module holds brother potential for reuse within ESTECO products. Additionally, ESTECO contributions to the MUSICODE OIMMP yielded the following KERs: enhanced understanding of BPMN applications in the OLAE domain; increased knowledge on the creation and deployment of cloud services; integration of modeFRONTIER[22] with the MUSICODE OIMMP via a web app.

Significance and novelty in relation to the state-of-the-art

Before the initiation of the MUSICODE project, Cardanit was the sole ESTECO product equipped with BPMN editing capabilities. The ESTECO BPMN editor, the software module developed during the project, makes it possible to add BPMN editing capabilities to any Angular web application, and can be easily extended to manage custom BPMN task. Leveraging this innovative software module, ESTECO successfully implemented the MUSICODE Workflow Editor and expanded Business Process Management (BPM) capabilities to VOLTA[23], ESTECO Simulation Process Data Management and Design Optimization platform. The VOLTA Modeler environment is built upon the same versatile software module that empowers Cardanit and the MUSICODE Workflow Editor with BPMN editing capabilities. The introduction of the VOLTA Modeler, complemented by the VOLTA Process Manager, positions VOLTA as a comprehensive and fully-fledged Business Decision Support System (BDSS).

Academic/Industrial market analysis and exploitation potential

With the newly incorporated BPM capabilities, VOLTA is poised to elevate ESTECO standing in the Simulation Data Management market, presenting a notable opportunity for increased market share. The introduction of the innovative VOLTA Modeler environment, powered by the ESTECO BPMN Editor, has swiftly captured the attention of the current client base, and is anticipated to unlock fresh sales opportunities by drawing in prospective customers. This strategic advancement positions ESTECO for both enhanced customer engagement and the exploration of new market segments.

Exploitation plan and expected results (1 year and 3 years after project completion)

ESTECO will assess the optimal utilization of the Workflow Editor verification module within its product offerings. As the module progresses to TRL 6 upon project completion, subsequent internal development efforts will be essential for seamless integration into VOLTA and Cardanit. The incorporation of BPMN verification and validation capabilities into the VOLTA Modeler holds the promise of simplifying interactions with executable BPMN models. This enhancement is anticipated not only to facilitate the use of VOLTA as a proficient business process orchestrator among its existing customer base but also to elevate its appeal within the market, making it even more compelling for prospective users.

[21] www.cardanit.com
[22] https://engineering.esteco.com/modefrontier/
[23] https://engineering.esteco.com/volta/

3.10 Organic Electronic Technologies (OET)

KER(s) obtained/developed in MUSICODE

Organic Electronic Technologies (OET) is a world leader in R2R manufacturing and technologies for flexible Organic Electronics (OEs) and holds more than 25 years' experience in thin film technologies. The value proposition of OET is related to production and design of OPVs and OLEDs. OET offers high quality OPVs and OLEDs in terms of efficiency and lifetime. Their OPVs have high transparency and are designed with high aesthetic regards. The integration of OPVs is easy no matter the surface (glass lamination, retrofit, ...) and the payback period is reduced.

Main activities of OET are:

- Manufacturing of large-scale Organic Photovoltaics with exceptional R2R printing processes enabled by unique laser patterning processes and in-situ characterization methods.
- Developing of custom R2R printing systems and in-line optical metrology tools and methodologies for the real-time monitoring of the nanolayer properties.

Significance and novelty in relation to the state-of-the-art

OET's expertise before MUSICODE includes:

- In-line & real time Metrology and Quality Control of OEs Processing & Manufacturing
- In-line Laser Patterning at low Temperature for Complex Free Form Designs
- In line Laser Processes P1, P2, P3 for Power Module Enhancement
- Automated Robotic Digital Cutting and Encapsulation systems for Mass OEs Production
- In-line R2R Inkjet printing systems design and development
- Automated Quality Control Platforms for implementing real-time decision-making processes in R2R industry (design and development)
- Automated printing 4-axis systems with monitoring control (design and development)
- Closed loop manufacturing with automated multi-axis coating station, camera monitoring and nondestructive metrology tools for real time quality control.

OET has leading performance in production and design of High efficiency fully printed OEs (OPVs and OLEDs) with R2R mass production capacity. Main advantages include the following:

- Attractive and Low-weight Form Factor, Flexible, Conformable.
- Simple, Cheap and Effective adaptation to any Surface.
- Freedom of Design, Free choice of colour palette to enable innovative and creative design.
- Tunable Optical transparency up to 40%.
- Efficient performance under Low Light and High Temperature conditions.
- Short Energy Pay-Back Time.
- Scalable and low-cost process, operating at low temperature.
- Patented technology and demonstrated in numerous applications.

MUSICODE targets to enable the Organic and Large Area Electronics Industry (OLAE), through the development of a novel Open Innovation Materials Modelling Platform, to expedite accurate and knowledgeable business decisions on materials design and processing for optimization of the efficiency and quality of OLAE device manufacture. The integration of sophisticated modelling capabilities allows OET to pioneer in OPV sectors by anticipating and solving challenges in OPV production, and other OEs, leading to the creation of superior products, that are not only more efficient but also more stable. This technological advantage positions OET as a leader in this emerging market, addressing the growing demand for integrated and sustainable energy solutions.

Main improvements due to MUSICODE up to now:

- **Improvement of production process, production yield and quality** of the final devices, due to the automated printing processes combined with the in-line metrology tools feedback.

Expected improvements:

- **Significant reduction in workload**, primarily by streamlining and simplifying the complex processes involved in the development and testing of Oes.
- **Reduction on fabrication expenses**, by enabling precise simulation and modelling reducing the need for extensive physical prototyping, thereby conserving resources, and reducing costs.
- **Optimized machine amortization** by improving the efficiency and efficacy of the manufacturing process, ensuring that equipment is used in the most productive manner, thereby extending its operational lifespan and maximizing return on investment.

Academic/Industrial market analysis and exploitation potential

OET has performed a thorough analysis of the global target markets where the MUSICODE innovations can be exploited. According to this, OET aims to promote OE products in Agrivoltaic, Building and Automotive markets for energy harvesting by exploiting the outcomes of the MUSICODE project concerning the improvement of production process, production yield and quality of the final devices. Opportunities arise from constantly increasing energy demand and EU commitment to Green Deal and zero greenhouse gasses emission by 2050. Also, more opportunities are coming from more environmentally friendly government rules, electrification of automotive industry and decarbonisation policy.

Predictions indicate that worldwide demand for Organic Photovoltaic Cells (OPVs) is expected to grow quickly in the coming years. This growth is mainly due to the widespread need for effective energy solutions and the rising demand for electricity. It is estimated that by 2028, the market value of OPVs will reach approximately 562.9 million euros, showing a steady increase at an annual rate of 13.5%[24].

Figure 3.2: Global OPV market forecast.

Agrivoltaics market is the most promising sector for the application of flexible Organic Photovoltaics. This market includes various types of greenhouses and is valued at 30.6 billion euros, expected to reach 47.1 billion euros by 2025. Agrivoltaics is a system that involves the simultaneous use of land for agricultural production as well as for photovoltaic production. Employing OPV for agricultural greenhouses is the key for a proper

[24] *["Global organic photovoltaics (opv) market report, history and forecast 2015-2026, breakdown data by manufacturers, key regions, types and application", 2020].*

market development of this PV-technology, since all the properties of OPVs, e.g. device flexibility, light weight, absorption range and ease of installation, are suitable for their integration. Using OPVs in greenhouses, and more particularly in Mediterranean Greenhouses which demand a lightweight structure for integration, can significantly save energy, grant autonomy, and increase production yield. Mediterranean Greenhouses market is valued at 14.7 billion euros and projected to grow to 22.1 billion euros by 2025.

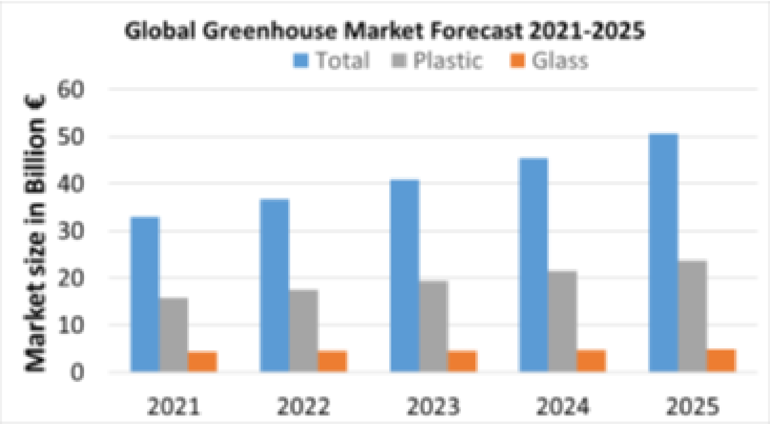

Figure 3.3: Global Greenhouse market forecast.

Building Market: Buildings are a major source of greenhouse gas emissions and energy consumption in the EU. They account for about 36% of emissions and 40% of energy use. The EU has set rules to improve buildings' energy performance, and by 2028, new buildings will need to include solar technologies. The BIPV market is expected to be enhanced by the growing interest in Green and Smart Buildings and the EU and government regulations (NZEB, European Renewable Energy Directive) that have created the regulatory framework for upgrade of existing buildings or new buildings that use renewable energy sources and have minimized energy costs. The flexibility and high semi-transparency of OPVs (>50%), make them candidate devices for integration in building elements such as windows, glass facades and skylights, offering high visibility and simultaneously energy efficiency. OPV integration in building elements where conventional, low-transparent, and heavy Si-based PVs cannot be applied, has the potential to convert buildings into energy harvesting units and reduce their carbon footprint. OPVs in buildings can be either built into new structures or added to existing ones, making renovations simpler. The BIPV market, including windows and curtains, is growing rapidly. In 2022, it was valued at approximately 12.83 billion euros and is expected to surge to 79.44 billion euros by 2030[25]. The glass BIPV segment alone is anticipated to grow from 2.02 billion euros to 4.67 billion euros during this period[26].

[25] *MarketsandMarkets, 2022, https://www.reportlinker.com/p05083038*

[26] *E. P. Anil Chaudhary, "Building Integrated Photovoltaics Market by Technology, Application, and End-Use: Global Opportunity Analysis and Indus," Allied Market Research,2021*

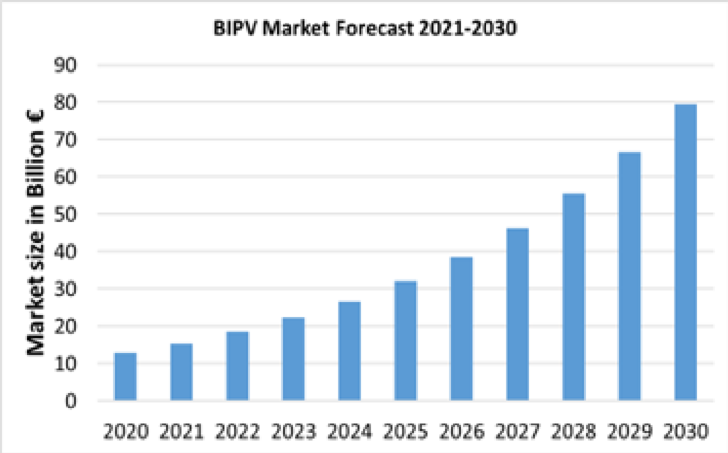

Figure 3.4: Global BIPV market forecast.

Automotive market: Vehicles contribute up to 12% of the EU's total CO2 emissions. To reduce this, alternatives to traditional vehicle power are becoming more popular, like electric vehicles (EVs). The lightweight and flexible OPVs can be seamlessly integrated on a conventional or electric vehicle, especially on the car's roof that covers a large area of the car, offering energy efficiency. The Solar EV market, currently valued at 0.4 billion euros, is projected to grow to 4.85 billion euros by 2030[27].

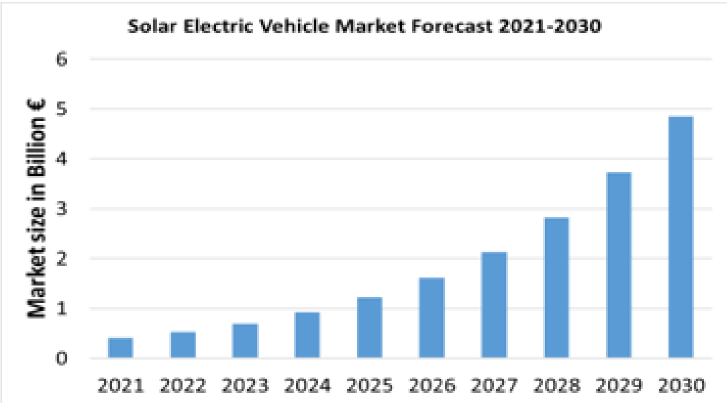

Figure 3.5: Global Solar EV market forecast.

Exploitation plan and expected results (1 year and 3 years after project completion)

OET targets to secure its know-how regarding the fabrication process of OEs gained during the implementation of MUSICODE by keeping it secret instead of publishing or describing it.

OET IPR strategy is based on:

- Information security and non-disclosure, agreements with employees, consultants, and subcontractors of the company (NDAs)
- Securing creative designs, new concepts and ideas filling i-depots
- Patent applications
- Business Model
- New publications

[27] *"Solar Vehicle Market 2021 to 2030," Precedence Research, 2021*

To reach the markets, OET has identified a market penetration plan consisting of the following steps:

Figure 3.6: Market penetration steps.

In the first step OET will leverage the interest through existing networks of collaborators (e.g. HOPE-A) and suppliers and will approach manufacturers and system integrators that could integrate OPVs in various applications. The main communication channels to reach the customer segments are identified as sales agents and representatives in high-potential markets. OPVs are planned to be sold to manufacturers for windows, building facades, automotive industry, and electrical engineering companies for BIPV applications,

During the second step OET will conduct dissemination activities and will launch initial reference projects to attract publicity and showcase its products.

In the third step OET will establish sales agreements with distributors, while implementing large-scale projects.

In the last step OET targets to enter joint venture agreements to establish production and logistics center and increase its marketing spending from its generated revenues.

Moreover, the commercialization strategy is expected to be supported by other projects as well. For example, OET is currently the coordinator of the ambitious Flex2Energy project, a 48-month project that aims to manufacture reliable Integrated Photovoltaics (IPVs) by developing an automated Roll-to-Roll manufacturing line for OPVs. Therefore, Flex2Energy will incorporate the novel results of MUSICODE (yield/quality improvements) and thus expand its commercialization pathways.

Based on the above, OET's roadmap for exploitation and commercialization is presented:

2021-2024: During this period, OET has been engaged with the reliable manufacturing of high-quality organic electronics in the R2R PPL at the LTFN facilities. The fabricated OPVs have been for the most part incorporated into small to medium scale demo projects. Moreover, during this time OET has been leveraging existing market interest and HOPE-A networks to attract interest from Building, Automotive and AgriVoltaics markets.

2025: Soon, the sales of OPVs fabricated by the R2R PPL will rise to about 2.000 m2/year. OET will invest in Business and Market Development and establish strategic relationships with partners in the EU, the USA, and Asia. The aim will be to develop AgriVoltaics, Building and Automotive Integrated pilot projects. Simultaneously, OET will be installing the 1st Mass Production IPV Machine, in the context of the ambitious Flex2Energy project.

2026: OET plans to have finalized the industrial-scale production line and increase its product annual sales to above 20.000 m2, with an annual production of more than 50.000 m2. Also, OET plans to invest in promotions and sales, by spending more than 10 % of its annual revenues on marketing, and to establish strategic partners and distributors networks worldwide. At this stage, OET will be targeting large projects to implement Building Integrated Organic PVs (BIPVs) and AgriVoltaics.

2027: With an established industrial-scale OEs production line, OET will reduce the production cost by increasing the production capacity to more than 200.000 m2 per year, while product sales will be above 70.000 m2 annually.

2028: By this time, OETs industrial production will have reached its full annual capacity of 1.000.000 m2. Further reductions in production costs will lead to product sales above 200.000 m2 per year. From this point on, OET will start investing in the development of new manufacturing lines.

3.11 AIXTRON SE (AIXTRON)

KER(s) obtained/developed in MUSICODE

The main KER developed in this project is advanced modelling of the OVPD deposition process as a function of reactor geometry and process conditions. This includes Computational Fluid Dynamics and Molecular Dynamics Calculations. These modelling results are used in combination with experimental deposition results. The modelling systems and boundary conditions started with a small, simple setup and expanded step by step to a more realistic scenario. As that the modelling could come closer to the reactor conditions it could be seen how the modelling could already replicate overall trends of experimental deposition rate results as a function of process parameters.

Significance and novelty in relation to the state-of-the-art

The results from the modelling are significant as more and more reactor conditions and molecular gas flow aspects can be considered. The experimental laboratory results in correlation with the modelling data can be used to sequentially improve the deposition process parameters for the fabrication of OE devices. Also improved designs and setups of OVPD deposition systems can be developed.

Academic/Industrial market analysis and exploitation potential

The potential becomes particularly significant as the research and development environment results from MUSICODE are being transferred to an actual industrial manufacturing area. For this it is also important to bring the new findings from the research and development size deposition areas to large area operation. This can help to satisfy the market need for high quality deposition on large areas to improve throughput, reduce production cost and to reduce energy consumption.

Exploitation plan and expected results (1 year and 3 years after project completion)

We see a wide potential field for exploitation of results in possible future gas phase deposition machines. It is planned to use new learnings from MUSICODE to develop new OVPD concepts. As the new advanced modelling concepts for improved system design, development and manufacturing are transferable to other gas phase deposition technologies they can be helpful also for other product lines of AIXTRON. In the next few years after project completion further efforts will be necessary to adapt the project results to advanced customer requirements regarding faster deposition process improvements and higher device quality.

4. Actions undertaken by the Consortium

To assist, accelerate and boost the sustainability and business planning of the MUSICODE project beyond the end of the project, UoI registered the project in 4 different modules. These are described in the next sections.

4.1. Horizon Results Booster, in Service 1, module C

This is a service provided for single projects having identified key exploitable results and a draft exploitation strategy. Dr. Manos Sofianopoulos was assigned as advisor from HRB. The steps taken thus far are:

a. A first meeting was held on 23/10/2023 between the advisor, E. Lidorikis and A. Laskarakis. The process was explained, and the required documentation and information needed from our side was explained. The 5 documents to be completed with information from our side include: 1. Exploitation intentions summary table, 2. Characterisation Table, 3. Risks_Assessment_and_Priority_Map, 4. Use options, 5. Exploitation Roadmap.
b. All partners collaborated to complete the 5 documents with requested information. These were sent to the advisor on 23/11/2023.
c. A 4-hour training meeting between the advisor and the partner representatives is scheduled for 12/01/2024, 12.00-16.00 CET, via Teams. A preliminary report for the project was prepared by the advisor (on 11/12/2023) and distributed to the partners.
d. The final report was returned to the project on 18/01/2024.

4.2. Horizon Results Booster, in Service 1, module A

This is a service provided for a group of EU projects sharing common technologies and similar objectives. The group of projects includes: OntoTrans, MUSICODE, NanoMECommons, CHARISMA, MatCHMaker, DOME 4.0. The lead is taken by partner IntraSoft of the DOME4.0 project. The steps taken thus far are:

a. Initial meeting with DOME4.0 and UoI on 25/10/2023. MUSICODE was presented and the two parties agreed on including MUSICODE in the project group.
b. 1st Group Meeting (zoom) with Project representatives took place on 08/12/2023 (12.00-13.00 CET). Introductions, short presentations, brainstorming on common collaborative activities, initial expectations, and preparations on working with HRB.

4.3. KETMarket GmbH & White IP Business Solutions

Will prepare an assessment of MUSICODE OITB results, business model and boundary conditions for sustainable operation after conclusion of the H2020 project. The objective is to gather all required results and information to enable KETMarket to prepare the MUSICODE sustainability concept and plan and suited legal structure. The scope of activities include:

a. Review of technical results, pre-defined business models and market potential based on previous project deliverables and the Grant Agreement.
b. Full stakeholder analysis and gathering of relevant legal information, constrains and business interest of potential members of the future OITB legal entity including:
    i. Survey to match the business interest of the members with the business model of the MUSICODE OITB.

   ii. Constraints arising from their legal nature (e.g. profit/non-profit) and ownership situation (e.g. public/private owned).
   iii. Conditions to be respected for collaboration with industrial customers including General Terms and Conditions, IP strategies, Data Protection, Specialty of Digital Services.

c. Initial business model workshop (1/2 day, online, inviting interested MUSICODE members) to create an updated business model canvas for MUSICODE and validate the business model.
d. Review against possible OITB business and sustainability models and identification of suited legal and operational models for MUSICODE.

The deliverables expected are:

1. Initial business model workshop.
2. Assessment report summarizing the key findings and giving recommendations on possible business and operation models.

The steps taken thus far are:

a. Initial meeting with KETMarket, WhiteIP, UoI and AUTh took place on 08/12/2023 (09.00-10.00 CET). Presentation of MUSICODE technology and objectives, discussion of collaboration objectives and expectations, information needed for them to start working.
b. NDA signed between KETMarket, WhiteIP and the MUSICODE consortium. E. Lidorikis signed on behalf of the consortium.
c. Supporting material (excellence part of the MUSICODE proposal, presentations, etc) were sent.
d. A 4-hour training session is scheduled for 20/12/2023, 13.00-15.00 CET.

4.4. University of Ioannina, Unit for Innovation and Entrepreneurship

This is an internal UoI service promoting exploitation of results and spin-out creations based on research done in the University (funded and non-funded). Steps taken thus far:

a. Initial call with the managing director of the Unit on 19/10/2023.
b. Completion of the Unit survey on 29/11/2023
c. Awaiting follow-up from the Unit.

Besides the 4 external modules described above, the partners held numerous internal meetings discussing the possible paths forward. The most important discussion items are:

a. Legal status of the entity to be formed.
b. Initial strategy to attract users and demonstrate a business case.
c. Partner involvement and status within the new entity
d. In-kind contributions from partners in the first 1-2 years

4.5. Next actions and steps

To facilitate an initial agreement, TinniT had drafted a preliminary MoU to serve as an initial basis for collaboration and planning for the legal entity to form after the end of the project. Also, a focused session on business development has been decided to occur live in Ioannina on 25/01/2024, the day before the Review Meeting with all partners present, where final plans and roadmaps will be decided. The Commercialization Roadmap decided in the M36 meeting will start materializing in the last year of the project. From the preliminary discussions between all partners this will involve several parallel avenues:

a. Finalize and sign an MoU between all partners interested in pursuing a commercialization activity.
b. Explore the legal options available, so that by M42 a concrete plan is in place.

c. Create demo video(s) and webinar(s) showcasing the MUSICODE platform.
d. Create a portal/platform where users can exchange info, request services, or offer support (including business-to-business interactions).
e. Showcase MUSICODE aggressively in EXPOs and Conferences.
f. Attract academic and industrial users with free support and services (including computing time) to create a first, and hopefully expanding, user and customer base.
g. Initial efforts to recruit the elementary personnel needed for the first years after the end of the project. This would be 2 technical and 1 managing position.

Explore options for seed funding sources (to support elementary key personnel and operations for the first 2 years after the end of the project), including “Angels”, European (e.g., “EIC *Accelerator*”), and other National, Regional, or Local sources.

5. Joint KER: the MUSICODE OIP

5.1 Description of the OIP

MUSICODE has built a unique Open Innovation Platform for Materials Modelling. The application area is Organic Electronics, for which the required modelling spans all length scales (electronic to continuum) and physics (quantum to fluid dynamics). The MUSICODE platform is a single-entry point for the industrial non-expert user, linked with data, protocols, editing tools, pre-templated modelling workflows and HPC facilities. It enables insight of how chemical structure, materials formulations, and process (gas/wet phase) conditions affect organic material properties and device performance. The MUSICODE platform offers key innovations on several levels, such as workflow design, data handling, software integration, HPC resource management, etc, making materials modelling accessible and user-friendly for industry in a level commensurate to engineering (continuum, finite element-based) software. The MUSICODE technology has already been demonstrated in the operational environment (TRL6).

5.2 Characterization of the OIP

Problem: The general problem is the difficulty industry (our potential customer) faces in integrating materials modelling and simulation (which is typically multiscale in nature) in their innovation process. The reason is the very high complexity and the high-end expertise needed, i.e., need to hire expert users (PhD level) for quantum or atomistic simulations, the need to find adequate computational resources (supercomputers), and to solve all licensing issues with the many different tools needed for multiscale simulations. To understand the throwback, consider in contrast the case of engineering simulations (e.g., finite-element-based structural mechanics, fluid dynamics and/or electromagnetics), for which there is usually a single multi-physics software needed, modest computational infrastructure requirements, and modest expertise needed by the user due to excellent GUIs. As a result, industry has, to a very large degree, integrated engineering simulation tools in their innovation process. This gap in adopting materials simulation in industry is the problem MUSICODE, targeting specifically the Organic Electronics industry.

Alternative solution: Most companies just rely on experimental trial-and-error processes. The problem with material simulations is that even if you overcome the initial steep learning curve, you still don't get exact quantitative answers due to the extreme complexity of the problems, i.e., thousands of randomly oriented molecules with quantum interactions between them. One still needs expertise to analyse results, find structure-property trends, and link with the experiments. This is opposed to engineering simulations at the continuum level which are highly deterministic and accurate. So, by and large, industry has avoided modelling for materials.

Unique Selling Point USP - Unique Value Proposition UVP: MUSICODE is trying to become the open window for a non-expert into the materials simulation world. It integrates under a single platform everything needed: models, data, workflows, solvers, infrastructure, expert support. Also, the platform will be open, from the point that external expert users will be able to link and offer expert translation support, data, and workflow design to industrial users. In effect, the vision is for MUSICODE to become a modelling Marketplace of its own where 3rd party expert users will be able to sell services and support to 3rd party industrial users utilizing 3rd party solvers and infrastructure. We believe there is no such structure/platform out there and there is really a need for one. Regarding what an industrial end-user will get out of the platform:

- *Knowledge building*: find data for materials, models, processes, experimental validation.

- *Translation*: find modelling experts to translate an engineering problem into a workflow.
- *Material discovery*: simulate different material structures and material formulations targeting specific material properties.
- *Manufacturing optimization*: simulate different process flows/conditions in manufacturing and linking them to material properties and device performance.
- *Prototyping*: find experimental experts and TestBeds to validate the simulation results and help with some testing and prototyping.
- *User friendly environment*: everything else (licenses, HPC infrastructures, etc) is already there.

Description: MUSICODE is an Open Innovation Platform for Materials Modelling, which integrates in a user-friendly way the data, models, licenses, infrastructure, and expertise needed, created a single-entry point for an industrial non-expert user. Being "Open" means that 3rd party expert users, software providers, HPC providers, etc, will also be able to provide support and sell services, making MUSICODE in effect a Modelling Marketplace in its own.

"Market" – *Target market:* The target industrial users are the ones using organic molecules and polymers in their products. In terms of industry sector, these are:

- Organic Electronic Material Industry
- Innovative Materials for Green Energy and Sustainability
- Healthcare, biosensors, and related systems

The customer segments are two:

- Expert users: offering data, new model APIs, new modelling workflows, translation services, and workflow design support for the non-expert users.
- Non-expert users: purchasing data and expert support, computing time, licensing, etc

"Market" – *Early Adopters*: In our case, we feel we have two types of early adopters:

- The expert users: invited to use the platform free of charge to create an expert community around the platform.

The non-expert users: invited to utilise what the platform has to offer free of charge to create a satisfied end-user community and ignite the first cooperation contracts.

"Market" – Competitors: There are few other platforms for materials modelling. For example, Aiida is an open one, offering an environment for quantum mechanical and atomistic simulations. However, it does not integrate data, workflow design, and HPC support in such a seamless way as MUSICODE, it is mostly a nice environment that expert users can facilitate their multiscale simulations in an efficient way, but still has roadblock for full adoption by non-expert users. Also, commercial solutions such as Materials Design, also offering quantum and atomistic modelling solutions. This is advantageous because there are no licensing issues (single license from the company is all is needed) and the front-end GUI should be very nice and intuitive. The weakness is that is it a commercial tool (more expensive), there can be no support from the greater academic community (which an Open Innovation Platform can ensure), and there is no integrated HPC support. A more detailed account of competitive platforms will be discussed in the next sessions.

Go to Market – Use model: Services, support, and contract research:

- Small subscription for data and support, pay-per-use for MUSICODE services (models, workflows, cpu time) and 3rd party HPC and solvers.
- MUSICODE as a service is free, but other tools will have a small fee based on the use.

Go to Market – Timing: We envision a 2-year period (the last of the project and 1 after) of networking and offering various services for free to create an initial user basis, including expert contributors and non-expert users/customers. This would mean the initial launch would be Jan 26.

Go to Market – IPR Background: No IPR will be used. The main platform infrastructure is the data management system (based on a commercial product of partner ANSYS), the workflow editor (based on a commercial product of partner ESTECO) and the interoperability layer (based on the open-source platform MuPIF offered by partner CVUT). Data, support, and expertise in workflow design and translation will not be covered by any IPR (trade secret), will be just part of the customer offer. A discussion has been made between the partners and a consensus has been more or less reached, that apart for the commercial tools already offered by the industrial partners, all other tools we would like to keep open-source, which will ensure that we can maintain a growing base of expert users and contributors and thus secure the sustainability and long life of the platform for the years to come.

Go to Market – IPR Foreground: No IPR foreground will be sought-after or used.

5.3 Novelty in relation to the state-of-the-art

From the point of view of simulation workflow design, the MUSICODE platform introduces a novel low-code approach based on the BPMN standard. Thanks to the Workflow Editor, expert users can turn MODA workflows into executable MuPIF workflows by designing BPMN processes. The Workflow Editor functionalities hide the complications of the standard and make it easy to design complex workflows. The automated translation process from BPMN to MuPIF Python code frees the expert users from having to know workflow implementation details. Finally, the Model Task element makes it possible to reuse models available on the platforms in different workflows.

Overall, there is no doubt that there is significant competition in the modelling market, as was shown in section 2. And that a much deeper due diligence it is needed from our side, i.e., allocating some funding to register, use, and evaluate the competitive resources. Having said that, there are several aspects of the MUSICODE technology and customer offer that are unique: One is the workflow editor directly coupled to a unique execution environment able to handle multiple HPC resources simultaneously. Another is the data constructions and ontology, allowing interoperability of data across different DBs and platforms. Another is the unique automatic data services and API architecture which allows model interoperability and easy integration of 3rd party models. As a whole, the MUSICODE platform novelty can be summed up to three key words: “open”, “interoperable”, and “reusable”.

Open: by construction, the workflows are open to interchangeable solvers through the novel data schemata and model APIs. Integration of 3rd party solvers and generally open-source solvers will attract multiple users. Also open is the support offered, having in mind that 3rd party experts and translators will be welcomed to operate through the platform and contribute to its value.

Interoperable: in terms of data and models. The target is for the workflow editor and data constructions through ontology to be so versatile that they break free from any restrictions imposed to other platforms.

Reuseable: again, in terms of data and models, where through the availability of data and models contributed by MUSICODE partners and 3rd party expert contributors, they can be reused by incoming new users.

The above are guaranteed not only by the expert partners of MUSICODE but also by the important cooperation initiated between the MUSICODE partners and other projects, entities, etc. To highlight a few, the OntoTrans collaboration on data interoperability through ontology, the OpenModel collaboration on new API development, the few new collaboration deals with industry (COATEMA, BrilliantMatters, etc).

5.4 Market needs and potential user base

Our reading is that the market needs versatile tools and expert support. The vision is to create an open platform that brings all these together. Open from the point of accessibility of course, not from the point that all data and knowledge created are open for all to see. This open platform should also attract 3rd party expert contributors which can create data and methods, offer models, build workflows, and support industrial users. In that sense, MUSICODE is open, it is not just selling something, but creating a common ground to foster innovation. The potential user base is depicted in Fig. 5.1.

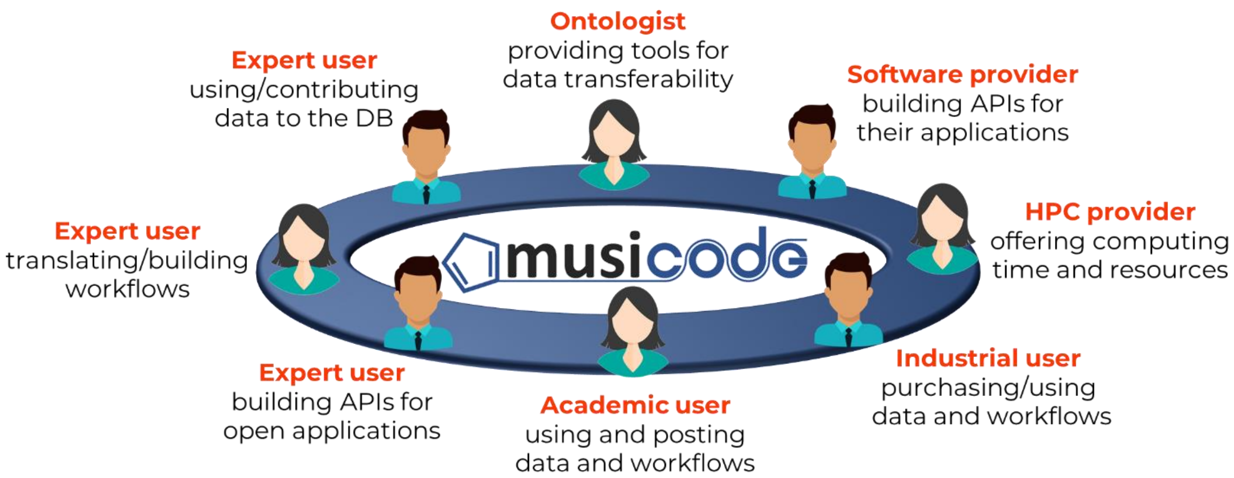

Figure 5.1. The envisioned user base of the MUSICODE Open Innovation Platform.

These include:

1. **Expert user translating/building workflows**: users creating and publishing reusable workflows, and/or providing services and support through the platform as a 3rd party expert. In exchange they receive recognition and compensation when providing support to 3rd parties.
2. **Expert user using/contributing data to the DB:** users using workflows and data from the database and posting their newly generated data. In exchange they receive recognition through the citations to their works.
3. **Expert user building APIs for open applications:** users creating models and model APIs either for their own solvers, or other open-source solvers. This can be also viewed as contract work for 3rd party industrial users requesting new specialized workflows.
4. **Ontologist providing tools for data transferability:** users contributing tools and interfacing with the data of the platform enabling automatic data transfer to/from other DBs and thus reusability of data.
5. **Academic user using and posting data and workflows:** users using the platform and publishing their results, creating new tools, and advertising value for the platform.
6. **Software provider building APIs for their applications: commercial software integrated on the platform and offered to customers on a per-use basis licensing scheme.**
7. **HPC provider offering computing time and resources:** public and private computational resources integrated on the platform and offered to customers on a per-use basis charging scheme.
8. **Industrial user purchasing/using data and workflows**: users seeking advice, support and ready to use data, models, workflows, and HPC infrastructures.

The above depicts an open collaboration and innovation environment, supported by a novel open innovation and discussion forum (to be built), where requests and offers can be made between the users. All activities and transactions are made through and facilitated by the platform, with the appropriate fee as a percentage remaining in the platform. All of this on top, of course, on expert support offered by the internal MUSICODE personnel.

5.5 Risk analysis

	Description of Risks	Critic-ality (1-10)	Proba-bility (1-10)	Risk Grade	Potential intervention	Interve-ntion success (1-10)	Action
	Partnership Risk Factors						
1	Disagreement on further investments: some partners may leave	*4*	*4*	**16**	As the actual investment needed is not large, the risk is mostly in terms of technology lost. However, there are redundancies between the partners	*9*	**Control.**
2	Disagreement on ownrship rules	*8*	*3*	**24**	Use of mediator to find mutual agreement	*5*	**Between Control & No Action**
3	Some partners don't want to contibute anything after the end of the Project	*3*	*8*	**24**	Other partners would cover these partners liabilities	*9*	**Control.**
4	Disagreement on the entity form, legalwise	*4*	*5*	**20**	Discuss other forms of legal entities	*4*	**No Action'**
5	Industrialization at risk: an business partner leaves the market.	*4*	*2*	**8**	Try and replace the partner internally or with the next best option.	*9*	**Control.**
6	Industrialization at risk: a partner declares bankruptcy.	*4*	*1*	**4**	Take over the partner's role internally	*9*	**Control.**
7	Partners break out and create competitive products	*6*	*3*	**18**	Ensure that all key technologies and practices are protected via exclusive agreements	*6*	**Control.**
	Technological Risk Factors						
8	Dependancy on specific wokflow editor	*4*	*4*	**16**	Make platfrom open to other editors as well	9	**Control.**
9	Dependency on the integration Platform	*9*	*1*	**9**	This would be difficult to solve, will have to adopt a new platfrom, which will take significant resources. However, the integration platform (MuPIF) is open source and community based, supported by the academic partner CVUT, who is dedicated to keeping supporting it.	*5*	**Between Control & No Action**
10	Data management solutions to complex to implement in an industrial environment	*2*	*2*	**4**	Upgrade DMS infrastructure and software	*9*	**Control.**
11	Worthless result: ill-timed disclosure.	*6*	*2*	**12**	I.e., some other very similar platform came out before ours. Reevaluate	*4*	**No Action'**

	Description of Risks	Critic-ality (1-10)	Proba-bility (1-10)	Risk Grade	Potential intervention	Interve-ntion success (1-10)	Action
					our value proposition and make necessary additions		
12	Worthless result: earlier patent exists.	*4*	*1*	**4**	Search the market prior of commercialization for patents infringements	*8*	**Control.**
13	Worthless result: better technology/methodology exists.	*9*	*2*	**18**	Reevaluate out value proposition and adjust	*5*	**Between Control & No Action**
	Market Risk Factors						
14	Value Proposition: Quality control and data management too expensive	*5*	*1*	**5**	explore web and cloud-based approach	*5*	**Between Control & No Action**
15	Insufficient penetration of the innovations in markets	*7*	*4*	**28**	Increase effort on dissemination and demonstrations in conferences etc	*3*	**No Action'**
16	Low capital availability to commercialize the results	*6*	*5*	**30**	Additional funding (e.g. customers, VCs, licensing, services, own resources etc.) will be mobilized to bring the MUSICODE innovations to TRL8-9	*6*	**Control.**
17	Exploitation disagreement: partners on the same market.	*6*	*1*	**6**	Work out a plan to aligned interests by negotiating roles and percentages	*4*	**No Action'**
18	Exploitation disagreement: partners with divergent interests.	*6*	*4*	**24**	Create opportunities for the partners to be more involve to the project. If not possible, activate/use the redundancies already in the projects	*7*	**Control.**
19	Worthless result: performance lower than market needs.	*8*	*3*	**24**	Reevaluate reasons for failure and push for better performance by adjusting modelling specs like tolerances, convergence criteria etc	*4*	**No Action'**
20	Nobody buys the product. Nobody needs it.	*9*	*3*	**27**	Advertise the product and establish a bullish period of offering free services to create a base of users. Use this base to advertise further the product	*3*	**No Action'**
21	Nobody buys the product. Too expensive.	*9*	*3*	**27**	Price adjustment	*6*	**Control.**
22	Nobody buys the product. Unsuitable sales force.	*9*	*7*	**63**	Hire personnel to create sales	*5*	**Between Action & Warning**
23	Nobody buys the product. The project hits against a monopoly.	*10*	*1*	**10**	Create synergies with the monopoly and try to cooperate with them	*3*	**No Action'**
24	Nobody buys the product. Problems at the time of the first sales.	*8*	*3*	**24**	Fix problems and boost sales with discounts on services	*5*	**Between Control & No Action**
25	Nobody buys the product. Rejected by end-users.	*10*	*3*	**30**	Create community of users and developers by offering free services, increase the value proposition with the new and improved products and go again with discounted offers	*4*	**No Action'**
	IPR/Legal Risk Factors						

	Description of Risks	Critic-ality (1-10)	Proba-bility (1-10)	Risk Grade	Potential intervention	Interve-ntion success (1-10)	Action
26	Legal problems: proceeding against us.	*4*	*2*	**8**	Ensure we are not infringing, correct any licensing issues, replace problematic tools/software with open-source ones.	*9*	**Control.**
27	Legal problems: we are sued for patent infringement.	*4*	*1*	**4**	Replace problematic tools with open-source tools	*9*	**Control.**
	Financial/Management Risk Factors						
28	The legal entity runs out of funds in a few years	*8*	*3*	**24**	Try to secure project funding for the entity.	*4*	**No Action'**
29	Weak exploitation: Inadequate business plan	*6*	*4*	**24**	Take steps to restart key aspects of the business to be more reliable	*4*	**No Action'**
30	Cannot find the appropriate personel for the business expansion	*8*	*6*	**48**	Change to remote personnel (online work) to get access to a larger pool	*7*	**Control.**
31	Know- how risks: there are leaks of confidential information.	*3*	*3*	**9**	Most of our platform will be based on open standards. In any case, if some "trade secret" is leaked: Identify the leaks, design improved services to keep having an added value over competition.	*7*	**Control.**
32	Multiple changes to original objectives.	*2*	*4*	**8**	While easy to adjust since all infrastructure is practically digital, still this can be a problem. So, focus efforts to finallize on a specific target.	*6*	**Control.**
33	Inadequate communication among partners.	*7*	*1*	**7**	Establish more focused and frequent communications.	*7*	**Control.**
34	Lack of endorsement from top management	*8*	*3*	**24**	Go to a spin-out solution	*7*	**Control.**
35	Off time supply of financial means.	*3*	*5*	**15**	Partners use their own means to support the platform at a minimum acceptable level until resources are supplied	*7*	**Control.**
	Environmental/Regulation/Safety risks:						
36	CO2 footprint per calculation	*1*	*5*	**5**	Search for approximations that will lighten the computational cost without sucrifying too much accuracy. In any case this will be required to also reduce the monetary cost of the calculations, as well as the return time.	*9*	**Control.**
37	Influence of laws and regulations.	*8*	*2*	**16**	Seek expert advice and correct/adjust operations	*5*	**Between Control & No Action**
38	Research is socially or ethically unacceptable.	*5*	*1*	**5**	Application domain does not have such issues. If the platform takes off and new application domains get enabled, then a policy of "proposal review" and ehtincs appraisal will be installed	*10*	**Control.**

A summary of all the above-mentioned risks and possible actions are visualized in the Priority map with risk numbers shown in Fig.5.2.

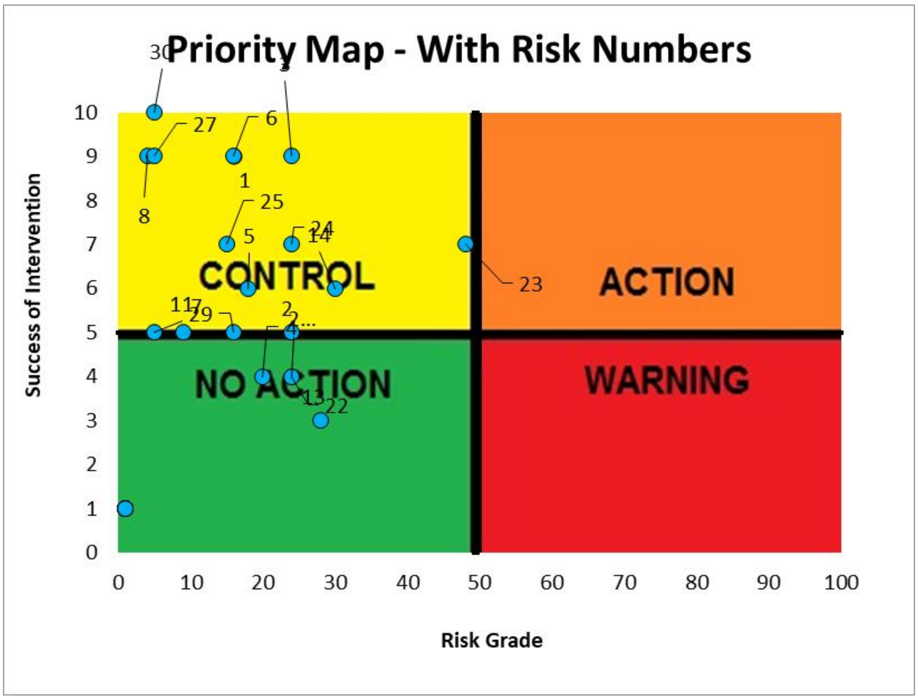

Figure 5.2. Priority map with risk numbers.

All risk factors present a low-risk grade coupled with a high probability of success of the planned remedy. A situation is defined where it would be preferable to keep an eye on what is happening (Control) to be ready to act. Most difficult risk is no.22 a market risk where if an unsuitable sales force is formed nobody will buy the product, that is there will be no enrolments in the platform. The probability and criticality seem to be high while the potential mitigation measures are difficult. This is a risk that should be looked at.

6. Long-term sustainability of key components

6.1 Data Management System and API for system integration

The data management system is currently implemented using Ansys Granta MI the market-leading material data management system. It offers a scalable solution to create, control and store valuable material data and is a commercial product supported by Ansys. However, it is also a highly configurable system which will need maintenance beyond the software, i.e. hosting, schema and data. Within the project the system is hosted and maintained by Ansys. Beyond the project there will be the need to negotiate license and training, according to the CA, with the legal entity continuing the operation.

The API for system integration is instead a prototype developed in research projects, mainly MUSICODE but with lesson learned for FORCE[28] and MarketPlace[29], and it would require additional development to increase the TRL. Currently Ansys is investigating the possibility to further develop the API internally with the objective to make it a supported tool. In this case the legal entity continuing MUSICODE could get is as the data management system, if this will not be the case there could be an agreement to provide the API "as it is" to the legal entity for further developments.

For both developments, frameworks such as the Ansys startup program[30] and/or the of Ansys partner ecosystem[31] seem viable options for the legal entity.

It is important to stress that the API allows the MUSICODE OIP platform to be flexible and modular. As all the integrations between the key software components happens through a solution agnostic REST API, these components could be potentially substituted by alternative software, with similar functionalities, reducing significantly technical risk for the sustainability for the platform.

6.2 Execution Layer - MuPIF

CVUT has developed and maintained MuPIF over the years. MuPIF is distributed under an open-source license. Even in a hypothetical case that CVUT steps out, this key component will still be available. The license permits anyone to continue its development and operation in the frame of MUSICODE or any other project, provided it follows the same license (LGPL). The only barrier is the needed expertise. During the project duration, many users, particularly from UoI and Tinnit became familiar with MuPIF philosophy and design and thus acquired the needed expertise. In any case, CVUT will continue to support development and operations after the end of the project. Once the legal entity is formed, it will add into the MuPIF developers, in addition to CVUT team.

6.3 Workflow Editor

The Workflow Editor is a web application based on the ESTECO BPMN editor, the core module of Cardanit, one of ESTECO commercial products. The ESTECO BPMN editor has been extended with the addition of a new element: the Model Task. Moreover, two modules have been implemented during the project to complete the application: the verification module and the export module. Both modules require additional development to increase the TRL. The Workflow Editor is hosted and maintained by ESTECO within the project. For user authentication, it connects to the platform single sign-on system, which is also managed and hosted by ESTECO. Beyond the project there will be the need to negotiate licenses and agreements, according to the CA, with the legal entity continuing the operation.

[28] https://cordis.europa.eu/project/id/721027
[29] https://cordis.europa.eu/project/id/760173
[30] https://www.ansys.com/startup-program
[31] https://www.ansys.com/en-gb/partner-ecosystem

ESTECO modeFRONTIER has been integrated with the platform and the integration of VOLTA is in progress. Both integrations make use of the platform single sign-on system and the data management system API and STK. They are hosted and maintained by ESTECO within the project. Plans for maintaining the integration of modeFRONTIER and VOLTA after the end of the project will be discussed.

6.4 Models and model APIs

UoI has established a model server at Ioannina, supplemented by massive storage. Both infrastructures will be supported by the UoI group during and after the end of the project, by own resources. This also includes development of new APIs and compilation of new workflows. The storage unit is destined to be the main dock for the data containers, alleviating pressure from the DMS and from ANSYS in maintaining it after the project. This yields the added benefit of the massive data containers being close to the model server where they are executed, minimizing communication latencies. Similar activity on a second model server will be undertaken in CVUT, thus a redundancy in infrastructures will ensure the uninterrupted use of MuPIF and execution of the workflows. In addition to server and storage, UoI will continuously offer a partition of the VIKOS supercomputer for free use (with quotas of course) by the incoming academic and industrial users.

6.5 Experimental validation

Expert academic users AUTh and USUR will continuously serve as open innovation test beds, offering support, advice, and validation services on materials formulation, process development, prototyping etc. Both partners have unique facilities for organic electronics, and thus will provide (through collaboration agreement) the ultimate benchmarking and validation services to potential users of the platform, as well as for the industrial user in general.

6.6 User support

Thanks to the Workflow Editor easy to use and friendly interface, a user new to BPMN can start modeling simple workflows in a short amount of time. As demonstrated in the project, a one-hour training session can be enough to provide a new user with the knowledge to create a new workflow, add Model Tasks and data elements, and export it to the DMS. Additional training sessions might be necessary for workflows involving loops and to learn about additional editing functionalities. ESTECO plans to add a documentation section to the Workflow Editor (based on Cardanit documentation, already available at https://www.cardanit.com/documentation/), example workflows will be made available after the end of the project. As for the training of new platform users, ESTECO can train within the project personnel of the legal entity that will oversee the onboarding of new users. As an alternative, ESTECO will evaluate the possibility to offer ad-hoc trainings for the Workflow Editor after the end of the project (ESTECO already offers BPMN trainings for Cardanit).

Other needs, such as user support for authentication (user credentials and management) and quality assurance (appropriateness of data posted, workflows published, etc) will be provided by UoI and CVUT using own resources, until the point that the new legal entity receives funding and/or creates its own revenue to support this.

7. Exploitation plan

7.1 General platform assessment

Musicode Platform combines elements of all three major platform types:

Marketplace:
Business model: Mediate transactions-based business for buyers and sellers and retain commission fee. Musicode example: SME and Industry buy modelling services, consulting, or computing time on the platform.

Community:
Business model: Provide an infrastructure for exchange, discussion, matching people and receive membership fees for access to the community.
Musicode example: Musicode brings together experts in different fields for joint research work (printed electronics, computing, modelling, process design).

Technology Platform:
Business model: Offers a technology platform (e.g. code base) for licensing.
Musicode Example: Musicode offers a technology and algorithms for material and process modelling in printed electronics.

To successfully implement a business model, MUSICODE shall select one of the three elements for a first business setup, which allows efficient implementation of a commercial business from earliest possible stage. **This is valid for the marketplace**. For this, a seller/provider side and a buyer side are required to be defined. This representation represents the starting point for the business, which can be expanded later. Such a construct for MUSICODE is depicted in Fig. 7.1.

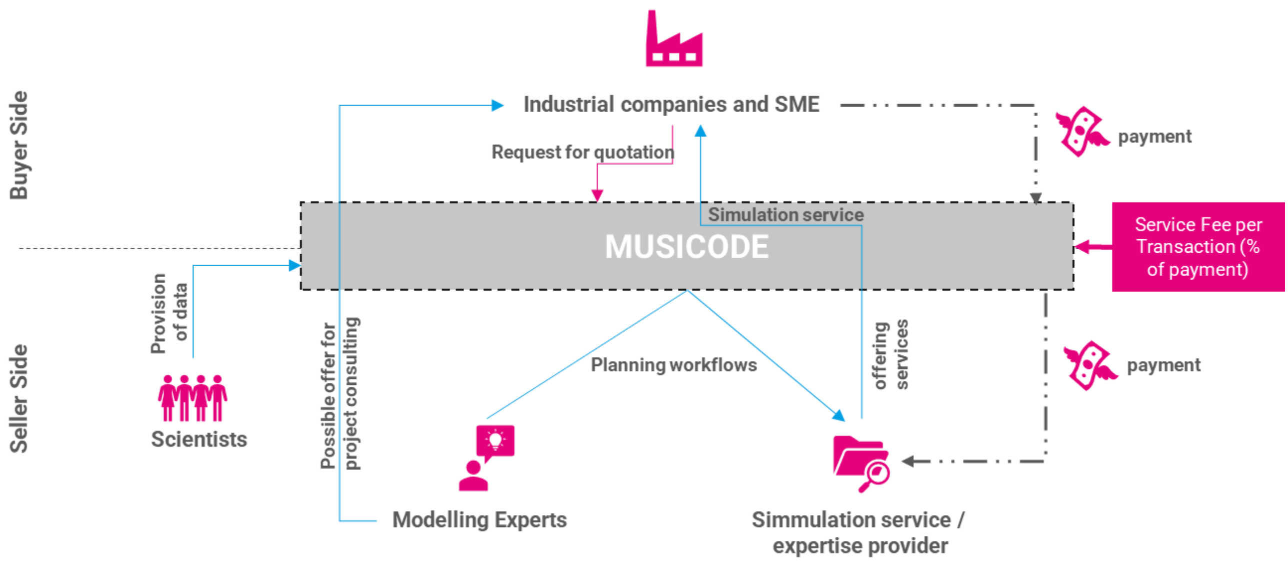

Figure 7.1. MUSICODE's Business Model as Marketplace for Modelling Services, Consulting and Computing time.

7.2 Business model canvas

The Business Model Canvas provides a quick and summarized overview of all relevant areas of the business model. For the MUSICODE platform it is shown in Fig. 7.2.

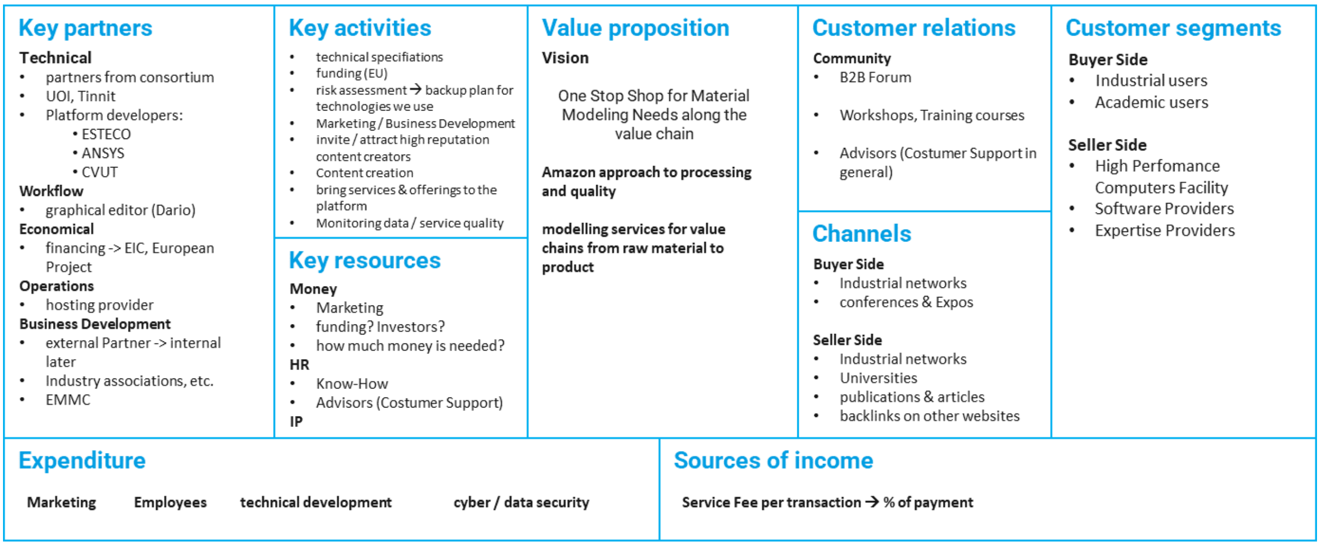

Figure 7.2. Business Model Canvas for the MUSICODE platform.

7.3 Value proposition

Regarding value proposition, these are summarized in Fig. 7.3 and 7.4 for the buyer side (comprises industrial users (SME) who are looking for solutions) and the seller side (comprises data providers and experts for solving the requirements of industrial companies), respectively. In Fig. 7.5 the customer relationship & sales channels are depicted.

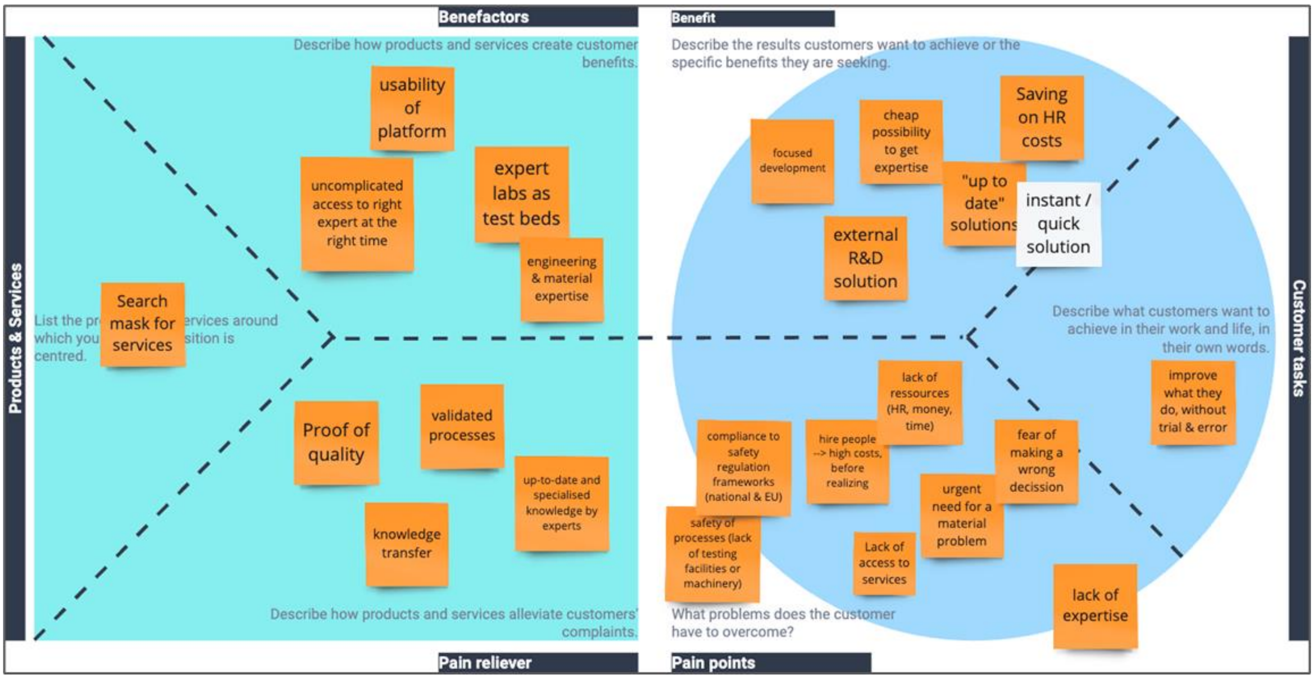

Figure 7.3. Value Proposition - Buyer Side Profile: comprises industrial users (SME) who are looking for solutions.

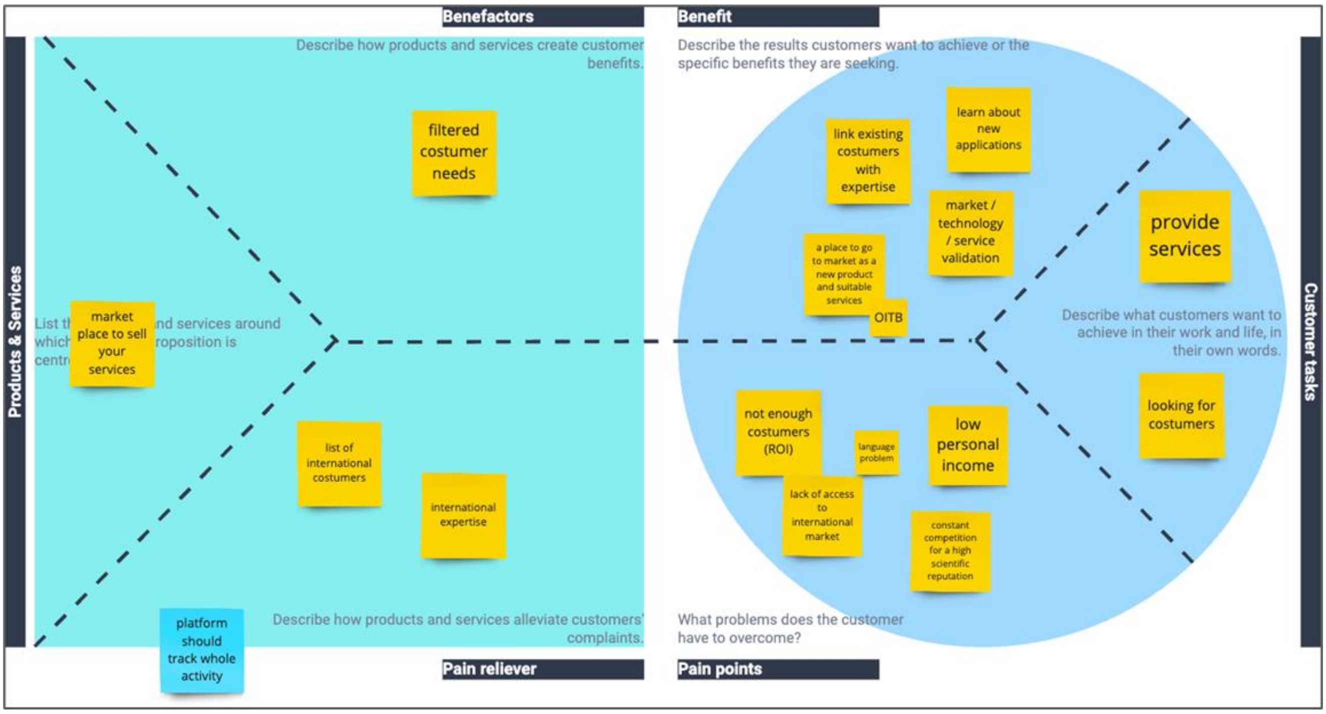

Figure 7.4. Value Proposition – Seller Side Profile: comprises data providers and experts for solving the requirements of industrial companies.

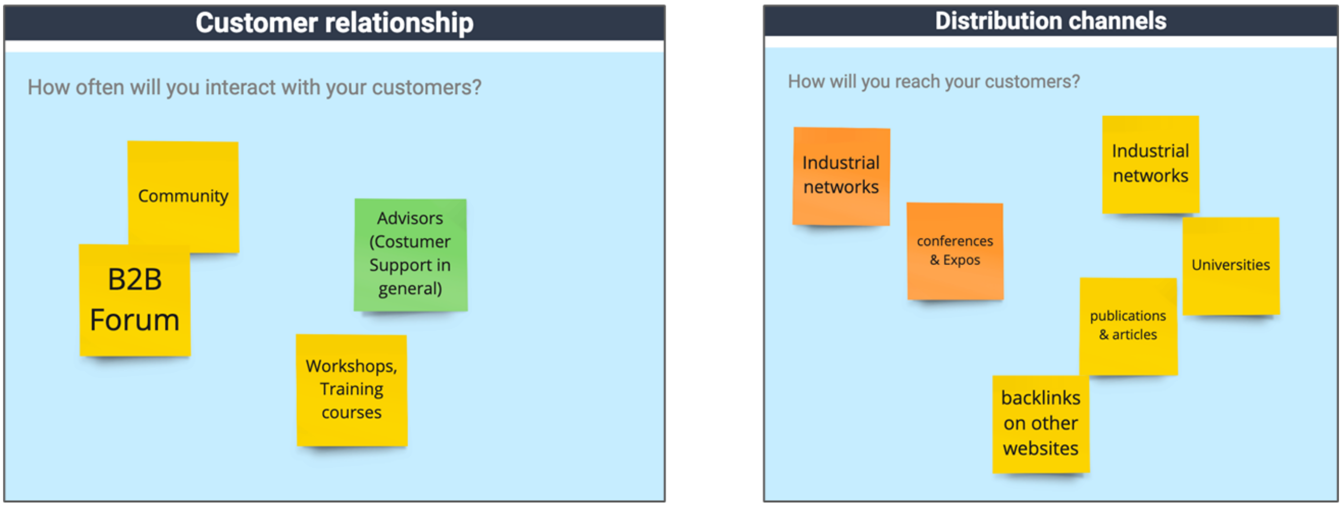

Figure 7.5. MUSICODE platform customer relationship & sales channels.

7.4 SWOT analysis

SWOT (strength-weakness-opportunities-threats) analysis serves as a guide to use strengths - reduce weaknesses - exploit opportunities - minimise risks. These are interrelated and interdependent, as explained in the graph shown in Fig. 7.6. The SWOT analysis applied to the MUSICODE platform is shown in Fig. 7.7.

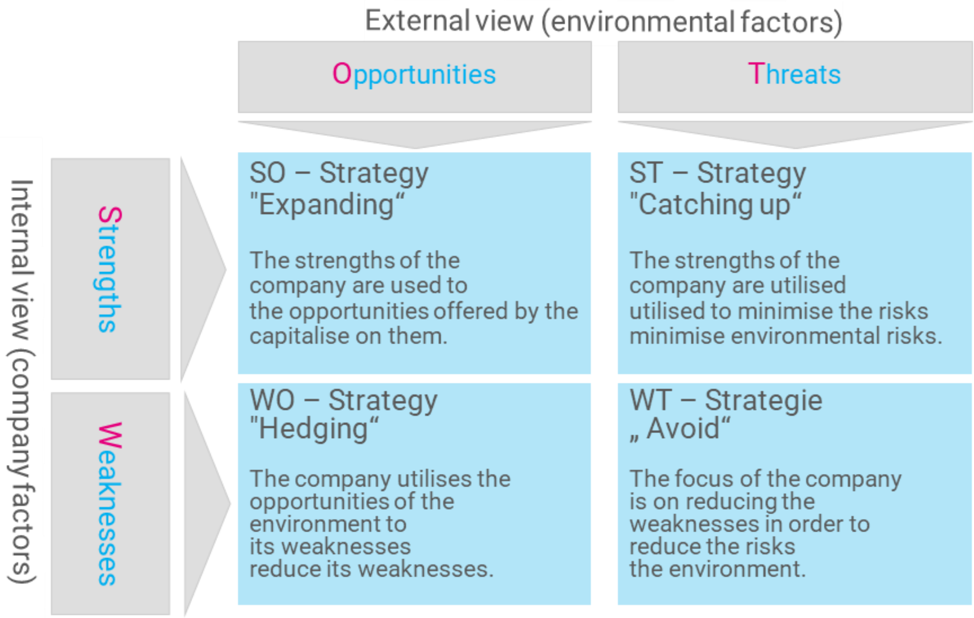

Figure 7.6. Principal targets and strategies involved in SWOT analysis.

Strengths	Weaknesses
• Front to market (technical) --> first mover • Pooling of expertise (academic world, industry, service providers) • Central database (open innovation) • Access to experts (provider side) • Network effects: The more users the platform has, the more valuable it becomes for each individual user • Scalability: The platform can often be scaled quickly and cost-effectively to serve a larger user base	• Lack of business experience / expertise • Lack of access to Buyerside • Product in need of explanation -> user does not immediately understand added value -> increased marketing effort • Business idea difficult for investors to grasp -> longer path to financing (very limited field of investors) • Dependence on user base: Success depends heavily on an active and growing user base
• Stage of Development of the platform • Green field for offer (many have failed) -> demand is the • Market expansion: Expansion into new markets and segments. • Innovative technologies: Integration of new technologies such as AI to improve services or offer new ones • Strategic partnerships: Collaboration with other companies can expand the offering and open up new customer segments • Change in user behavior: An increasing willingness of users to use platform services (e.g. online shopping)	• Platform relies on Granta MI product from ANSYS, risk if Ansys drops off and quits collaboration so that Granta MI is not available any more • Legal and Contractual limitations with public entities as suppliers may apply (e.g. universities may be required to contract end-user (buyer) directly • Service provider does not provide desired quality -> bad "publicity" (minimization by QM representative) • Risk of running out of money during development • Risk that companies (buy-side) bypass the platform • Data protection concerns: Growing concerns about data protection and data security can affect user confidence
Opportunities	Risks

Figure 7.7. MUSICODE platform SWOT analysis.

7.5 Exploitation roadmap

The exploitation roadmap, starting on Q1 of 2024 includes the following:

Actions: The first actions to be done include:

- Establish the legal entity,
- Increase market penetration by offering demo use of the product to clients,
- Promote the product to conferences and exhibitions,
- Resolve any issues with license etc.

Roles: The initial planning and distribution of roles include:

- UoI and AUTh will coordinate the actions.
- UoI, ANSYS, ESTECO and CVUT maintain the platform infrastructure.

  - UoI offers CPU time, data storage, and expert support.
  - ANSYS maintains the database and user authentication.
  - ESTECO maintains the workflow editor.
  - CVUT maintains MuPIF and with UoI the connections to 3rd party HPCs.
- TINNIT and FLUXIM offer their commercial software through the platform.
- USUR and AUTh serve an experimental Open Innovation Test Beds.
- All partners promote the product in conferences.

Milestones:
1-2 months -> Establish legal entity and resolve issues with software license (first MS).
3-4 months -> Offer demo version to potential clients.
4-6 months -> Promote product to conferences and exhibitions.
11-12 months -> Have at least 2 customers who use the product.

Financials Costs: Cost estimation to implement planned activities (1 year, 3 years). These are just estimates, we'll need to do some research to get better values:
- Expenses for the establishment of the entity (legal fees, etc) (<10 k€)
- Cost of the demo free services (mostly personnel) (<15 k€/Year)
- Travel costs for promotion (<10 k€/Year)

Other sources of coverage: The resources needed to bridge the investment needed to increase TRL and ensure the result is used. The platform will reach TRL7 by the end of the project. The main resources that will be needed to reach even higher are only personnel. Typical ways to do that is use expert personnel already employed in the universities, expert students already supported by other projects, and 3rd expert academic users that become contributors in exchange of some of the tools and infrastructure (e.g., part of the UoI HPC cluster) offered for free.

Impact in 3-year time: The impact in terms of growth/benefits for the society. The best way to describe the impact that MUSICODE can in principle create for society is by considering the huge impact engineering software (like ANSYS, COMSOL, etc) have in industry already. This means more jobs, faster time to market, better products, more sustainable productions methods, less materials waste.

7.6 Key partnerships with 3rd parties

Required key partnerships are the ones with HPC facilities. Currently we have 4 HPC partnerships including the internal UoI resources. Images of the facilities are shown in Fig. 7.1.
- KAROLINA peta-scale supercomputer (IT4Innovations, 2023) served by IT4Innovation supercomputing center, being the part of the European HPC resources provided by European High Performance Computing Joint Undertaking (Euro HPC Joint Undertaking, 2023).
- MELUXINA peta-scale supercomputer (573 nodes, ~0.2 Pflops), funded jointly by the EuroHPC Joint Undertaking, through the European Union's Connecting Europe Facility and the Horizon 2020 research and innovation programme, as well as the Grand Duché du Luxembourg.
- ARIS supercomputer (532 nodes, ~30 Tflops), served by GRNET High Performance Computing Services (hpc.grnet.gr), part of PRACE, HPC-Europa and the European Leonardo Consortium.
- MUSICODE internal computational resource, i.e., the VIKOS supercomputer (~1000 cores, ~2.5 Tflops) maintained by UoI.

Figure 7.1. The HPC facilities already linked with MUSICODE and willing to provide service.

More details on 3rd party HPC integration can be found in deliverable "*D5.3 Connection with 3rd party HPCs and customer offer*". The immediate action for MUSICODE is to demonstrate good usability of these infrastructures by users, before extending to more HPC partnerships.

Other key partnerships include projects and entities already cooperating with MUSICODE on technology aspects of the platform, e.g., OntoTrans, OpenModel, EMMO, etc.

7.7 Current status on exploitation

MUSICODE's dissemination activities have attracted significant interest, resulting in the first pool of industrial users already being formed. Specifically:

- Cooperation agreement with R2R machinery developer COATEMA GmbH, Germany (Fig. 7.2). Interest is in the CFD workflow on the dryer chamber. Details of the actual work are confidential. An NDA has already been signed with TinniT is providing the expert support.
- In principle cooperation agreement with organic materials developer Brilliant Matters, Canada. Initial demo workflows on materials properties and calculations are being developed by UoI for them, with the aim to result in a collaboration contract.
- Expression of interest to collaborate with ELORPrintTec-Facility for Printed Electronics, a Research Center of Excellence in the University of Bordeaux, France. This is one of the top European institutes on Organic Electronic and a possibility to establish firm collaboration would be invaluable.

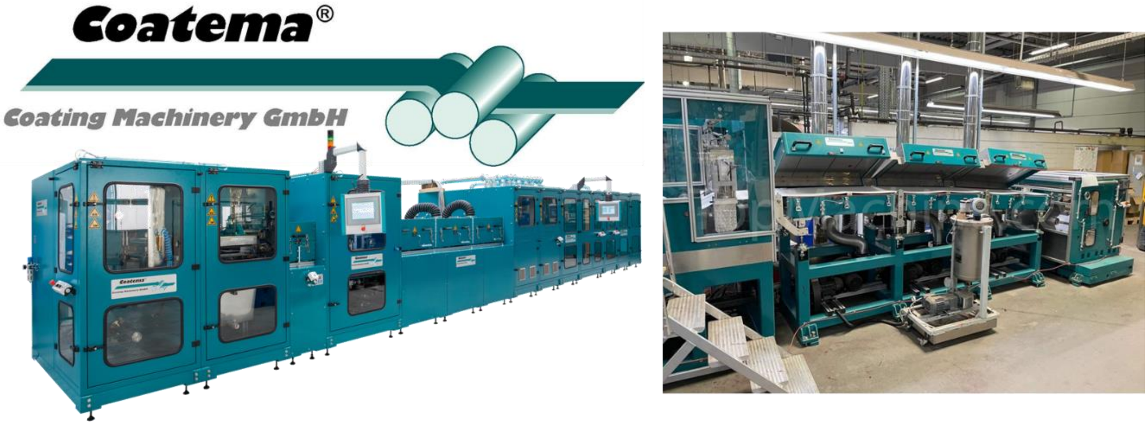

Figure 7.2. COATEMA GmbH, a Coating Machinery Manufacturer, already working with MUSICODE to improve its dryer chamber designs.

7.8 Sources of income and 3-year projections

Funding: Explore sources of funding that can support activities for the immediate period after the end of the project. These include:

- EIC Accelerator project (addressing SMEs at high enough TRL).
- Angel Funding.
- Participation in new HE projects as an SME.

Revenues: Projected revenues and eventual profits once the KER will be used (1 and 3 years after use). Using very rough and conservative estimates, just to put some numbers down: assume an industrial user spends about half the cost of a medium level employee (i.e., ~20 k€/year). Of this, about 80% goes for 3rd party licensing & computing time, and 20% stays as profit with the platform. Then:

- After 1 year: 10 users, ~200 k€ total expenditure, ~40 k€ platform revenue (no profit).
- Break-even: 20 users, ~400 k€ total expenditure, ~80 k€ platform revenue. Considering 2 full-time personnel (~60 k€/Year) and ~20 k€ other operational costs, the platform is barely sustainable.
- After 3 years: 50 users, ~1,000 k€ total expenditure, ~200 k€ platform revenue. Considering 4 full-time personnel (~120 k€/Year) and ~50 k€ operational & advertising costs, the platform is profitable.

The above is estimated as revenue on top of the activities of the internal personnel of the platform. That is, it is expected that part of the salaries will be covered by services and support offered to customers by the platform expert personnel. In general, we estimate that anything above 20 users should make the platform profitable. However, we stress that all this requires some more due diligence from our side.

Other sources of revenue: A small annual subscription fee for users is also possible. However, this should be implemented after a sizable pool of users is created. Also, depending on the size of the user base, hosting advertising on the website and open forum might also create a sizable income for the platform. Both these are, however, understood that will come into effect once user numbers are significant.

8. Conclusions

The strengths, weaknesses, opportunities, and risks were defined and analysed. A realistic plan forward towards establishing a legal entity in the form of a spin-out is presented, including strategies to attract funding, financial estimates, and forecasts, etc. Importantly, first feedback from potential industrial customers is very encouraging with initial collaborations are already being agreed. Given the status of the project, i.e., completed its 3rd year and entering the last, this is indeed the right time to kick-start the exploitation and commercialization effort: activities are still funded under the project, improvements in technology are continuously implemented, and operations are still risk free. The plan forward is concrete and steps to be taken clearly defined. Hopefully, the commercialization attempt will be successful, and the Business Plan update at the end of the project will involve a new legal entity having formed.