



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)

Grand Agreement: 953187

Project Start Date: 01/01/2021

Project Duration: 48 months

Deliverable 2.8

Report on seamless coupled devices/module simulations

Date: 14-09-2023



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

Project co-funded by the European Commission within Horizon 2020 Research and Innovation Programme		
Dissemination Level		
PU	Public	
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)	x

Deliverable author(s): Sandra Jenatsch, Fluxim AG

Contributors: Name(s), Organization(s)
Antonio Cabas Vidani, Fluxim AG

Draft Revisions: v1.1 submitted to coordinator on 13/09/2023
v2.0 approved on 14/09/2023

Copyright

@ Copyright 2021-2024 The MUSICODE Consortium

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 UK (ANSYS)	UK
	AIXTRON (AIXTRON)	Germany

This document may not be copied, reproduced, or modified in whole or in part for any purpose without written permission from the MUSICODE Consortium. In addition to such written permission to copy, reproduce, or modify this document in whole or part, an acknowledgment of the authors of the document and all applicable portions of the copyright notice must be clearly referenced.

All Rights reserved.



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"

"The European Commission support for the production of this publication does not constitute an endorsement of the contents which reflects the views only of the authors, and the Commission cannot be held responsible for any use which may be made of the information contained therein."

Contents

Publishable summary	4
1. Introduction	5
1.1 Objectives of WP/Task.....	5
1.1 Purpose of this Document	5
2. Methodology and results	6
2.1 Methodology	6
2.1.1 Device scale simulations.....	6
2.1.3 Large-area simulations	6
2.1.4 Coupling between 1D device scale and 2+1D large-area simulations.....	8
2.2 Results	8
2.2.4 Large-area device and module simulations.....	8
2.2.4.1 Link between device and module level (Laoss – Setfos integration)	8
2.2.4.2 Application example 1: DC and AC response of single-carrier device with defects	12
2.2.4.3 Application example 3: Module design simulations.....	15
3. Discussion	22
3.1 Achievements	22
3.2 Risks	22
3.2 Next steps	22
4. Conclusions	22
References	22

Publishable summary

This document reports the work carried out in the Task 2.4 “Device and module modelling (M1 – M36)” under the WP2 “Development of multiscale modelling tools (M1 – M36)”. WP2 develops modelling tools from micro-, to meso- and macroscale to simulate fabrication processes, material parameters and device performance of OE materials and devices. Task 2.4 focusses on opto-electronic simulations of thin film multi-layer device and large-area (including module) simulations. In collaboration with the partners, Fluxim adapted and extended its commercially available simulation tools Setfos and Laoss to improve the models and facilitate a satisfying user-experience.

This report shows the modelling work undertaken in Task 2.4 since the last deliverable report D2.2. The title of the deliverable “seamless coupled devices/module simulations” was technically already implemented in the commercial simulation software Laoss, version 4.1. This module was released in May 2021 and the concept was therefore already presented in D2.2. In this report, the integration is briefly repeated and two examples of simulations spanning the 1D electro-optical (“Setfos”) and the large-area (“Laoss”) device level are explained. Finally, an update on module simulations in collaboration with the University of Surrey is presented.