



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 6.4

Validation of modelling gas phase processing in OE materials

Date: 20-01-2024



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): P. K. Baumann (AIXTRON/APEVA)

Contributors (only the lead contacts during the preparation of this document are identified herein)

Name	Organization
P. K. Baumann	AIXTRON/APEVA
C. Trapalis, E. Lidorikis	Uoi
A. Kneer	TinniT

Draft Revisions: 18/01/2024 version v1.0 sent to coordinator
20/01/2024 version v2.0 approved by the coordinator

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 (USUR)	UK
	Aristotle University of Thessaloniki (AUTH)	Greece
	Czech Technical University in Prague (CVUT)	Czechia
	Fluxim AG (FLUXIM)	Switzerland
	TinniT Technologies GmbH (TINNIT)	Germany
	ANSYS UK (ANSYS)	UK
	Esteco SPA (ESTECO)	Italy
	Organic Electronic Technologies (OET)	Greece
	APEVA SE (APEVA)	Germany
AIXTRON SE (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 Purpose of this document	5
2. Methodology and results	6
2.1 OVPD reactor and fabrication of organic material layers	6
2.2 MD deposition statistics - sticking coefficient.....	10
2.3. CFD modelling of molecular deposition	14
3. Conclusions.....	18

Publishable summary

The MUSICODE modelling platform is used to simulate a gas phase deposition system and processes to fabricate organic electronic material layers. The organic material is transported in a heated inert gas stream through the hot deposition system under vacuum conditions and gets deposited uniformly on a cold substrate. Computational Fluid Dynamics and Molecular Dynamics Calculations are used to try to match the experimental molecular deposition of the gas phase deposition process.