



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 6.3

### Report on dopants in OE material mobility (modelling and validation)

**Date: 28-02-2024**



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):** D. Kutsarov, University of Surrey (USUR)

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

Name	Organization
V. Appuhamilage, D. Kutsarov, R. Silva	SURREY
A. Paliagkas, E.Doudis, A.Laskarakis	AUTH
K. Kaklamanis, M. Andrea, K. Kordos, D. Papageorgiou, E. Lidorikis	Uol
S. Jenatsch, C. Vael-Garn	Fluxim
V. Kyriazopoulos	OET

## Copyright

@ Copyright 2021-2024 The MUSICODE Consortium

Consisting of Coordinator:	University of Ioannina (Uol)	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
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
Glossary .....	5
1 Introduction.....	6
1.1 Purpose of this document .....	6
2 Methodology .....	7
2.1 Validation methods .....	7
2.2 Modelling methods .....	8
2.2.1 Device scale simulations.....	8
3 Results and analysis.....	10
3.1 Experimental studies .....	10
3.1.1 Fabrication and characterisation of small-area OE devices .....	10
3.1.2 Fabrication and characterisation of large-area OE devices.....	12
3.2 Modelling studies .....	21
3.2.1 Optical modelling of OPV devices.....	21
3.2.2 Electro-optical modelling of non-doped and doped devices .....	23
3.2.3 Fitting doped single-carrier devices with a full device model.....	24
3.2.4 Microscopic modelling of doped OPVs.....	28
4 Discussion .....	31
4.1 Achievements .....	31
4.2 Risks .....	31
4.3 Next steps.....	32
5 Conclusions.....	32
References:.....	34

## Publishable summary

This document outlines the progress achieved in modelling and analysis of the doping effect in OE materials and devices. Special attention is given to the influence of the doping on the physical properties of OE materials, such as alteration of the charge carrier mobility. The modelling data generated by UOI and FLUXIM is based on the experimental input provided by AUTH, OET, and USUR. This report is a continuation of the activities reported in D6.1. Results included in this document show the successful fabrication, characterisation, and modeling of PCDTBT- and PBDB-T- based HOD doped (and not) with F4TCNQ. Herein, trends of measured JV key figures from pristine and doped devices could be reproduced by device simulation. Additionally, optical, and structural characterization of doped PBDB-T and PBDB-T:BTP-12 layers were carried out. Ultimately, hole mobility values from PCDTBT and PBDB-T were extracted. Furthermore, the effect of using F4TCNQ as a dopant material for PBDB-T:BTP-12-based OPVs was studied showing an OPV device performance improvement with the increase in dopant concentration up to a certain threshold. Modelling results of carrier mobility as a function of doping concentration are shown for the PCDTBT:F4TCNQ and IDIC:BV systems using multiscale charge transport simulations.