EMERGE
Emerging Printed Electronics Research Infrastructure

D5.6

2nd Interim report on modelling and simulation of processes, devices and systems FLAPEP connected

WP5 Access to design, modelling and simulation

The EMERGE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement Nº 101008701

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List of abbreviations

BHJ – Bulk HeteroJunction
CAD – Computer-Aided Design
DD1D– One Dimensional Drift Diffusion modelling
FLAPEP – Flexible Large Area Printed Electronics and Photonics
FZJ – Forschungszentrum Jülich / Helmholtz Institute Erlangen-Nürnberg
GIWAXS – Grazing Incidence Wide Angle X-Ray Scattering
HMU – Hellenic Mediterranean University
JOR – Joanneum Research
JV curve– Current-Voltage curve
NFA – Non-Fullerene Acceptor
OSC – Organic Solar Cells
PDI – perylene-diimide
RISE – Research Institute of Sweden
SEM – Scanning Electron Microscopy
SME – Small & Medium Enterprise
TA – Transnational access activity
TUD – Technische Universitaet Dresden
UNOVA – Instituto de Desenvolvimento de Novas Tecnologias (UNINOVA)
VPI – Vapour Phase Infiltration
WP – Work package
WUT – Warsaw University of Technology

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CONTENTS

Contents

The EMERGE project has received funding from the European Union’s Horizon 2020 research and Innovation programme under grant agreement Nº 101008701

1. Executive Summary

This document gives an overview of the incoming projects that required modelling and simulation activities (TA1.2) offered by the EMERGE consortium between June 20th, 2023 and June 20th, 2024.

There have been nine projects project proposals formally requesting modelling and simulation activities (TA1.2) in the last year of the EMERGE project. One project has been rejected. For three of them (all projects requiring joint modelling and experimental activities), TA1.2 modelling activity was actually not expected (project owner's mistake/misunderstanding at submission) or has not been implemented (lack of time/priority). Among the five accepted projects really requiring TA1.2 activity, four were pure modelling projects, only one a joint modelling/experimental project.

The projects are all related to ideas with very low degree of maturity, mainly submitted by experienced researchers of academic institutions. Personal communication between EMERGE project partners and applicants still remains the most effective dissemination tool at this stage.

Three projects have been implemented in this time period, remotely, by the EMERGE partner FZJ itself, as a simulation service. Together with the previously completed projects (see deliverable D5.5), FZJ implemented five projects and JOR one project. Two accepted projects are to be implemented soon by FZJ and JOR, respectively. The implementations have been very successful: the results are in-line with the expectations, the projects owners foresee a significant impact of the results in terms of product or publication.

The main concerns regarding TA1.2 activities are still the low number of incoming projects, as well as the maximal project duration which is too short for these low-maturity topics and might discourage submission.

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2. Introduction

This document aims at giving an overview of the incoming projects that required modelling and simulation activities (TA1.2) offered by the EMERGE consortium in the last year of the EMERGE project (30/06/2023-30/06/2024). This is an interim report on the project status to date (30/06/2024).

3. Overview of EMERGE projects requesting TA1.2 activity

The table below summarizes the general information on the incoming projects.

To date, there have been **nine project proposals** requesting modelling and simulation activities (TA1.2) during the 4th-9th EMERGE calls.

- Five of them were submitted during the 5th call (submission 01/07/2023-30/09/2023),
- whereas three of them has been submitted during the 6th call (submission 01/01/2024-31/01/2024),
- and one has been submitted during the 8th call (submission 01/03/2024-31/03/2024).

Regarding the status:

- Four projects have been implemented (5th call)
- One project has been rejected (5th call)
- Four projects have been accepted but not implemented yet (6th and 8th calls)

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Call	ID	Title	Previous proposals	Author	Nationality	Type of institute	Country/ Home institute	TA(s)	Pretended Institution(s)	Status	Comment relative to TA1
5	**6398**	Understanding the morphological instability of bulk heterojunctions in organic solar cells based on polymer/fullerene blends	-	**Gitti Frey**	Israel	University	Israel / Technion - Israel Institute of Technology	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems**	**FZJ**	Completed	PFSimProst @FZJ
5	**6426**	Correlating processing-morphology-performance of high efficiency organic solar cells (OSCs)		**Gitti Frey** Sasha Simotko	Israel	University	Israel / Technion - Israel Institute of Technology	**TA3. Prototype fabrication** TA1. Theory: Modelling, simulation, and design of materials, devices and systems	**FZJ**	Completed	DD1D @ FZJ
5	**6427**	Dopant variation for controlled doping of the active layer in vacuum evaporated solar cells	**4074**	**Mathias Nyman**	Finland	University	Finland / Åbo Akademi University	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems** TA4. Characterization of prototypes and demonstrators	**TUD**	Completed	Nothing implemented regarding TA1
5	**6435**	Study of electrodes' surface modification effect with new perylenediimide derivatives	-	**Beata Luszczynska** Bartosz Orwat	Poland	University	Poland / Lodz Uniwersity of Technology	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems** TA2. Material synthesis and ink formulation	**FZJ** **TUD**	Completed	DD1D @ FZJ
5	**6436**	Ternary Mathematics Its Principles and Solutions Offered (refractive index and polarization)	-	**Ruslan Pozinkevych**	Ukraine	University	Eastern European University	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems****	**WUT**	Rejected	NA
6	**6470**	Training and basic knowledge on OPV and OLED manufacturing.	-	**Marc Vizern** Ferran Micaló	Spain	SME	Spain (EU)	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems** TA3. Prototype fabrication	**HMU**	Accepted (after revision)	Nothing required regarding TA1
6	**6471**	Formation in the design, printing and validation of biosensors	-	**Ferran Micaló** Marc Vizern	Spain	SME	Spain (EU)	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems** TA3. Prototype fabrication	**JOR**	Accepted	Learn how to design screen-printed biosensors (not sure they'll use modelling...) @JOR
6	**6474**	Design and Simulation of Efficient Interfacial Layers for Hybrid Solar Cell Applications	-	**Khuram Ali** Zohaibali	Pakistan	University	Pakistan	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems**	**FZJ** **RISE**	Accepted	DD1D
8	**6525**	Simulation of a photoplethysmography (PPG) sensors system in a cardiological medical device	-	**Johannes Gladisch**	Germany	SME	Sweden (EU) / Acorai	**TA1. Theory: Modelling, simulation, and design of materials, devices and systems**	**JOR**	Accepted	Raytracing optical simulations, S/R optimization of LED/PD system for PPG sensors @JOR

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4. Analysis of incoming proposals

4.1. Overall information

Among the nine projects, five have been submitted by EU citizens/institutions, three by EU-close citizens/institutions (Israel, Ukraine) and one by Asian citizens/institutions (Pakistan). Beyond this, we can see some trends appearing regarding the institution, gender, experience of the project owners:

- Six of the nine projects have been submitted by academic institutions, whereas only three projects comes from Small and Medium companies.
- The project owners are dominantly experienced researchers (University professors-scientific coordinator, middle-aged scientists, managers). Only one primary project owner is a post-doc. A few secondary project owners are post-doc, PhD student, technician, respectively.
- No significant gender trend, even if there are more male applicants: four project owners are female and six are male.

Regarding the requested EMERGE institution for the modelling part, four projects have been requesting FZJ-activities, two JOR-activity, one WUT-activity, one TUD-activity and one HMU-activity. For TUD and HMU who do not offer modelling services, it looks like the project owner misunderstood the adequation between TA offers and their project. To date, only the partner UNOVA did not receive activity requests for modelling and simulation.

Interestingly, the degree of maturity of all projects has been evaluated by the project owners as very low / prospective idea (“Basic idea” or “Proof of concept”).

4.2. Focus on publicity

The origin of the project proposals is various:

- Five of the seven project owners have become aware of EMERGE by word of mouth, direct contact or discussions with the EMERGE partners. For now, personal communication still seems to be the most efficient method for advertising EMERGE. Only two of the project owners knew about EMERGE through social media / website.

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- Note that two project owners submitted two distinct projects, whereas one project owner submitted a follow-up project (No 6427) of a previously completed EMERGE project. This proves positive regarding the attractivity of the EMERGE approach.

This is in line with the overall picture of all EMERGE project proposals.

4.3. Focus on the requested TA1 activity

Four of the projects were pure modelling projects, and five of them formally required joint modelling and experimental activities. In practice:

- **TA1 modelling activity has not been implemented / is actually not expected for four of them**, either because they have been rejected (project 6436), or because the activity has been formally required but actually not planned (projects 6427, 6470, 6471). In the latter case, TA1 activity were mentioned in the proposal as joint/secondary activities together with experimental activities. This highlight the need for more clarity in the submission process on which activities the user should require.
- **Five projects really require TA1 activity**.
    - Four of them focus on printed solar cells (6398, 6426, 6435 and 6474). Three of them required electro-optical modelling of the cell behaviour (FZJ). The last project (6398) required simulations of process-structure relationships in solution-processed electronics using the in-house simulation code PFSim-Prost (FZJ).
    - The last project focuses on a medical sensor system and requires modelling of the sensor's optical behaviour by JOR (project 6525).

5. Overview of completed projects

In this section, we provide a quick description of the results obtained for the three completed projects involving TA1 activities. Note that the completed project 6427 is not considered here since no TA1 activity was actually involved.

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5.1. Summary of objectives and results, potential use after project

5.1.1. Project "Understanding the morphological instability of bulk heterojunctions in organic solar cells based on polymer/fullerene blends" (6398)

- Objectives: the bulk heterojunction morphology (BHJ) of a polymer-fullerene organic solar cell (OSC) has been observed by scanning electron microscopy (SEM) after vapour phase infiltration (VPI). The BHJ shows nicely an amorphous donor-acceptor phase separation and subsequent acceptor crystallization upon thermal annealing. The objective of the EMERGE project is to combine advanced simulation methods with the already provided images to provide a full understanding of the temperature-dependent phase evolution of polymer-fullerene blends. To this end, the experimentally observed morphologies will be reproduced using phase-field simulations. Then, based on these simulations, the physical mechanisms responsible for morphology evolution will be identified and extensively analyzed.
- Results: The experimentally observed morphologies have been successfully reproduced using the PFSimProst framework, in particular the amorphous phase-separation prior to fullerene crystallization. Not only the thermodynamics, but also the kinetic mechanisms/properties leading to such a behaviour have been identified.
- Potential use after the project: this data most likely will lead to the publication. The results represent a basis for the analysis of further material systems, and the approach might be generalized for a predictive understanding of morphology evolution under thermal loading.

5.1.2. Project "Correlating processing-morphology-performance of high efficiency organic solar cells (OSCs)" (6426)

- Objectives: The general objective is to understand the morphology formation and the structure-property relationship of a novel high-efficiency non fullerene acceptor (NFA) OSC system, PM6:Y6, by correlation of SEM images, optoelectronic measurements and simulations. While the VPI-SEM measurements are performed at the project owner's lab, the objective of this EMERGE project is the printing and characterization

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of the corresponding full solar cells stacks, as well as the simulation of their optoelectronic behaviour with drift-diffusion simulations. The processing conditions are varied in order to obtain a full process-structure-property relationship.

- Results: films and solar cells using PM6:Y6 as a transport layer have been characterized and fabricated, respectively, and the sensitivity to the process parameters have been identified. The JV curves have been successfully fitted by drift-diffusion simulations.
- Potential use after the project: the data will most likely be used for a future publication. Use the knowledge gained by imaging, simulations, and device measurements to further improve device performance towards Flexible Large-Area Printed OSCs.

5.1.3. Project "Study of electrodes' surface modification effect with new perylenediimide derivatives" (6435)

- Objectives: The main aim of the project is to deepen the knowledge of the interactions between different layers of organic solar cells (OSC) to optimize the devic. To to this end, an electrode-modifying interlayer based on perylene-diimide (PDI) derivatives is introduced between the ink-jet printed metal and the OSC active layer. In the EMERGE project, the objective is to identify the role of the PDI layer on the device physics using drift-diffusion simulations, based on the model parameters required to match the experimental JV-curves. Guidelines for the optimization of OSCs with the use of PDI-based cathode interlayers should be formulated with the help of the simulations as well as of GIWAXS measurements.
- Results: The experimental JV-curves of solar cells without and with PDI interlayer have been successfully simulated, showing what physical mechanism is responsible for the performance improvement. The sensitivity to the properties of the interlayer have been investigated, providing design rules for optimization of the full solar cell stack.
- Potential use after the project: the data will most likely be used for a future publication. The results can be used to robustify/identify stack design rules of general validity for solar cells.

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5.2. Realized vs. expected

For all three projects, the work realized was not fully in-line with expectations, due to lack of time and technical difficulties. Typically, the necessary resources to perform the tasks have been underestimated, so that the effort represented significantly more than expected (projects 6398, 6426), or that not all the planned simulations have been performed (project 6435). Despite of this, even in the latter case, the objectives of the projects could be reached successfully.

5.3. User feedback

Unfortunately, the user feedback on the completed projects is not yet available. It will be dicsussed in the next report on “Modelling and simulation of processes,devices and systems FLAPEP connected”.

6. Conclusion

As a conclusion, a small number of projects (nine) requesting modelling and simulation activities (TA1.2) have been submitted during the third year of the EMERGE project. Modelling still remains a minor topic as compared to experimental projects, as expected. The option to require joint modelling/experimental activities helps increasing the number of TA1 projects. However for these joint projects, modelling is secondary, and at the end sometimes not implemented. Modelling might even not be needed but nevertheless required, due to frequent mistakes on requested activities at project submission (project insufficiently precisely defined, misunderstanding of the offer catalogue, bad knowledge of offered techniques and EMERGE partners capabilities). It might be helpful to improve the description of the EMERGE offer, and in any case previous discussions of EMERGE partners with the project owner beforehand are crucial for proper project definition.

To date, among the six projects involving TA1.2 activities that have been completed since the beginning of EMERGE (including those mentioned in deliverable D5.5), five have been implemented remotely, by the EMERGE partner FZJ, as a simulation service, and are related to printed solar cells. The last one has been implemented by JOR. Remote implementation seems to be an appropriate approach for theoretical activities, as well as the

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implementation by the EMERGE partner itself if the simulation tool requires advanced, timely training.

All these modelling activities have been judged successful by the project owners, and in some cases the collaboration was pursued beyond the EMERGE project itself. This shows the relevance of the investigated topics, but also that the maximal project duration (10 days) is insufficent to answer the scientific question of the project owner. This is understandable considering that all incoming projects handle very low maturity, research-oriented topics, which might be hard to structure in very time-limited sub-projects.

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