D5.3: Theory Transnational Access Provision

WP5. TA1 – 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

FLAPEP - Flexible Large-Area Printed Electronics and Photonics

FZJ – Forschungszentrum Jülich GmbH

GWP - Global Warming Potential

HI ERN - Helmholtz Institute Erlangen-Nürnberg for Renewable Energy

HMU – Hellenic Mediterranean University

JOR – Joanneum Research Forschungsgesellschaft mbH

OPV – Organic Photovoltaics

LEH - Light Energy Harvesting

TA – Transnational Access Activities

TA1 – Access to design, modelling and simulation

TLO – Technical Liaison Office

TUD – Technische Universität Dresden

RISE – Research Institute of Sweden

SME – Small Medium Enterprise

UoA – Units of Access

UNOVA – Instituto de Desenvolvimento de Novas Tecnologias (UNINOVA)

WP – Work package

WUT – Warsaw University of Technology

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1. Executive Summary

The deliverable 5.3 – Theory Transnational Access Provision belongs to the Work Package 5 (WP5) titled as TA1 – Access to design, modelling and simulation.
The purpose of this report is to provide a comprehensive summary of the proposals related to TA1 which were submitted during the first five calls of EMERGE, that is, from the beginning of EMERGE project in June 2021 (M1) to December 2023 (M30).
Overall, ten proposals were submitted on the EMERGE website requesting theorical access provision. Three projects were successfully completed and five are currently under evaluation. Two were not suitable for Theoretical Access Provision and were carried out at different Transnational Access Activities (TA). Besides that, six proposals were initially submitted for different TAs but were also included theorical activities (TA1) during the project execution.

2. Proposals

2.1 Concluded proposals

Three projects were submitted for Theory Transnational Access Provision, and were successfully completed by the end of 2023. Project 3829 was carried out in person at JOR, while the activities from projects 3832 and 3833 were done remotely at FZJ. Table 1 brings the details about each project such as the title, project call and the period of implementation.

Table 1: List of projects submitted for TA1 and concluded by M30.

Call/ Proposal ID	Project Title	EMERGE institution	User type of access	Period of project implementation
2nd Call 3829	Uniformity in visual appearance of individual cells in laminated OPV devices	JOR	**In-person**	**Start date:** 20-03-2023 **End date:** 31-03-2023
2nd Call 3832	High-throughout exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films	FZJ	**Remote**	**Start date:** 23-01-2023 **End date:** 27-01-2023
2nd Call 3833	High-throughout exploration of crystaline phase diagram	FZJ	**Remote**	**Start date:** 27-03-2023 **End date:** 31-03-2023

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	space for the accelerated design of organic thin films			

Project 3829 was submitted by Hassan Abdalla, an Austrian Product Manager who works at the Small Medium Enterprise Epishine located in Sweden. Epishine is an energy impact company, reimagining the capture of light with market-leading printed organic solar cells. It has 15 products already on the market with the aim to make electronics sustainable, for people and planet.

Both projects 3832 and 3833 were applied by the same user, the Professor Olga Wodo. She is a Polish Professor-scientific coordinator at the department of Materials Design and Innovation at University of Buffalo in the United Stated of America. Her research focuses on in-silico studies of the morphological phenomena in engineered and natural heterogeneous systems with application to several engineering systems such as organic solar cells (which was the focus of her research through EMERGE). Table 2 summarises information about the users.

Table 2: Information about Users who carried out concluded projects which were originally submitted for TA1.

Call/ Proposal ID	User (nationality)	Research role	Home Institution (Country)	Type of Institution
2nd Call 3829	Hassan Abdalla (Austria)	Product Manager	Epishine (Sweden)	SME
2nd Call 3832	Olga Wodo (Poland)	Professor-scientific coordinator	University of Buffalo (USA)	University
2nd Call 3833				

Proposal 3829: Uniformity in visual appearance of individual cells in laminated OPV devices (JOR)

- Objectives: In this project an approach should be developed to use extrinsic measures to reduce the visual differences between cells in an organic solar cell and inhomogeneities on the active area by means of diffusive surfaces and patterns, exploiting also optical effects on a microscopic level but keeping the output power as high as possible. Subsequently, the approach should be validated both theoretically and experimentally. Only approaches that can potentially be scaled up to a cost-effective R2R production will be considered.

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- Requested TA/installations: Design, modelling and simulation (TA1), Demonstrator characterization and validation (TA4)
- Used TA/installations: Modelling & simulation (1 UoA), Device metrology & characterization (5.5 UoA)
- Results: The main achievements of the theoretical and experimental work were the knowledge that it is possible to change the reflection spectrum of the Light Energy Harvesting (LEH) module by inserting a coloured foil between the cells and the backsheet. This gives the possibility to change the visual appearance of the LEH modules without losing efficiency. In addition, it is possible to reduce the angle-dependent inhomogeneities with a coloured front foil that has high transmission values. This leads to less efficiency losses when using such a front foil.

Proposal 3832: High-throughout exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films (FZJ)

- Objectives: The scope of the proposed work includes the generation of a library with 245 ternary phase diagrams for amorphous blends consisting of polymer, small molecule, and solvent. The library will become the input to machine learning pipeline to (i) illustrate the alternate approach for screening of materials based on the phase diagram characteristics and (ii) to facilitate the discovery of the design rules of material selection for organic thin films, including flexible electronics. The library will be used to perform clustering analysis, and then mapping them back to the design space. The mapping back will inform the design rules for solvent selection. In the longer perspective, this work has the potential to accelerate identifying solvent additives for champion Organic photovoltaics (OPV) systems.
- Requested TA/installations: Design, modelling and simulation (TA1)
- Used TA/installations: Design, modelling and simulation (1 UoA)
- Results: The generation of three libraries with 245 ternary phase diagrams each for amorphous blends consisting of three compounds: polymer, small molecule, and solvent. Three configurations were screened: (i) polymer-small molecule-solvent, (ii) small molecule-small molecule-solvent and (iii) small molecule-solvent-solvent. The design space of interaction parameters was defined and sampled to provide the data for the clustering. Data has been generated by HI ERN group, and subsequently

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analyzed by the user at her home institution. As a result, the initial design rules for the amorphous ternary materials systems were derived.

Proposal 3833: High-throughout exploration of crystalline phase diagram space for the accelerated design of organic thin films (FZJ)

- Objectives: The scope of the proposed work includes the generation of a library with 405 temperature-dependent binary phase diagrams for polymer-small molecule blends.The library will become the input to machine learning pipeline to (i) illustrate the alternate approach for screening of materials based on the phase diagram characteristics and (ii) to facilitate the discovery of the design rules of material selection for organic thin films, including flexible electronics. The library will be used to perform clustering analysis and then mapping them back to the design space. The mapping back will inform the design rules for solvent selection and derive the design rules for acceptor and donor blends. In the longer perspective, this work has the potential to accelerate identifying materials (small molecules and conjugated) for champion OPV systems.
- Requested TA/ installations: Design, modelling and simulation (TA1)
- Used TA/ installations: Design, modelling and simulation (1 UoA)
- Results: The generation of six libraries with 405 temperature-dependent phase diagrams each for crystalline binary blends. Three configurations were screened: (i) polymer- solvent, (ii) polymer-small molecule and (iii) small molecule-solvent. For each configuration two cases were considered, where either the first or the second component crystallizes, while the other is amorphous. In each dataset, it was screened five-dimensional input space with the following material properties varied in the range with three sampling levels: interaction parameter between components, the heat of fusion of each component, the melting temperature of each component. Data has been generated by HI ERN group, and subsequently analyzed by the user at home institution. The user is currently working on learning the design rules for the binary crystalline-amorphous materials systems.

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2.2 Submitted Proposals Currently Under Evaluation

During the EMERGE 5th Call, five proposals (6398, 6399, 6427, 6431 and 6434) were submitted requesting Theory Transnational Access Provision, and they are all currently under evaluation. Four of them were applied by universities while one from SME (Small Medium Enterprise). Moreover, three institutions are from the European Union (two from Finland and one from Poland) while one is from Israel and another one is from Turkey. Table three brings information about the proposals mentioned above.

Table 3: List of proposals submitted for TA1 access to the EMERGE infrastructure in 2023 which are under evaluation.

Call/ Proposal ID	Proposal title	Home Institution (Country)	Type of Home Institution	Pretended EMERGE institution(s)
5th Call 6398	Understanding the morphological instability of bulk heterojunctions in organic solar cells based on polymer/fullerene blends	Technion - Israel Institute of Technology (Israel)	University	FZJ
5th Call 6399	Point-of-care (PoC) Nanoplasmonic biosensor chip integrated microfluidic device for pathogen detection	Xfold Imaging Oy (Finland)	SME	JOR RISE
5th Call 6427	Dopant variation for controlled doping of the active layer in vacuum evaporated solar cells	Åbo Akademi University (Finland)	University	TUD*
5th Call 6431	Patient-Specific Numerical Modeling in Palliative Solutions for Infants with Dependent Pulmonary Blood flow.	Istanbul Medipol University (Turkey)	University	FZJ RISE
5th Call 6435	Study of electrodes' surface modification effect with new perylenediimide derivatives	Lodz Uniwersity of Technology (Poland)	University	FZJ TUD

*Although TUD is not formally a WP5 member, one project was submitted requesting TUD as hosting partner for theory access provision. The TLO will decide if the project will be reassigned to other TA or if another partner from WP5 will host it.

2.3 Proposal submitted to TA1 but reassigned to other TAs

Two proposals were submitted requesting Theory Transnational Access but were reassigned to other more suitable Transnational Activities after the evaluation from the TLOs. Proposal 4010 (3rd Call) was carried out at Materials Characterization and Industrial Printing utilities from WUT, and proposal 4070 (3rd Call) was done using Vacuum deposition equipment at TUD. Table 4 summarizes the information about the reassigned projects.

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Table 4: List of proposals submitted for TA1 access to the EMERGE infrastructure from 2021 to 2023 but were approved for other TAs access.

Call/ Proposal ID	Proposal title	Home Institution (Country)	Type of Home Institution	EMERGE Institution	Reassigned Transnational Activity
3rd Call 4010	Thin and flexible electrodes for capacitance measurement	Innovation Partners (Europe) AB (Sweden)	SME	WUT	Materials characterization (TA2.1) Industrial Printing (TA3.3)
3rd Call 4074	Controlled doping of the active layer as a way of enhancing performance of organic solar cells	Åbo Akademi University (Finland)	University	TUD	Vacuum deposition (TA3.2)

2.4 Proposal submitted to other TAs but requiring TA1 during implementation

From the beginning of EMERGE project in June 2021 (M1) to December 2023 (M30), six proposals were initially submitted for different TAs but were also included theorical activities (TA1) during the project execution. Four projects were carried out at RISE (ID 4625, 5682, 5814, 5827), one at JOR (ID 3986) and two at WUT (ID 4001 and 5826).

Table 5: List of projects originally submitted to other TAs but reassigned to TA1 during project execution.

Call/ Proposal ID	Proposal title	Home Institution (Country)	Type of Home Institution	EMERGE Institution	Original Transnational Activity Requested
3rd Call 4001	Formulating screen printing ink/paste application for resistive heater application	Levidian Nanosystems Limited (United Kingdom)	SME	WUT	Device Preparation (TA3.1) Materials characterization (TA2.1.) Chemical & physical techniques (TA2.2.)
4th Call 4625	Mass production of NFC tags printed on paper with additive techniques and at least 2 years lifetime, easy to recycle.	ROTIMPRES (Spain)	SME	RISE	Industrial printing (TA3.3.) Validation and standardization (TA4.2.)
4th Call 5682	Evaluation of scalability of 2D printing of magneto-rheological and magneto-electrical composites	Fundación BCMaterials-Basque Center for Materials, Applications and Nanostructures (Spain)	RTO	RISE	Functional 2D & 3D printing (TA3.2) Device metrology & characterization (TA4.1)
4th Call 5814	Screen-printed structures of alternating TiO2 and CeO2 layers used as an oxygen-sensing materials	Institute of Chemistry, Technology and Metallurgy (Serbia)	RTO	RISE	Industrial printing (TA3.3) Materials characterization (TA2.1)

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4th Call 5826	2D/3D CELL-PILs for tissue engineering	NOVA FCT (Portugal)	University	WUT	Industrial printing (TA3.3.) Materials characterization (TA2.1.)
4th Call 5827	Manufacturing and Characterization of Flexible Thermoelectric Modules and associated electronics through printing techniques	ParsNord Thermal Comfort ApS (Denmark)	SME	RISE	Device Preparation (TA3.1.) Device metrology & characterization (TA4.1)

3. Summary of simulation softwares used

The theoretical models of Project 3829 were simulated on Matlab Software while the projects 3832 and 3833 used the Phase-Field Simulations of Process-Structure relationship (PFSim-Prost) and In-house FZJ-DCFI modelling tool for solar cell JV-curves simulations.

All projects carried at RISE have accessed Computer-Aided Design (CAD) through Adobe Illustrator for screen printing. At projects ID 4625, 5682 and 5814 the software was used for the design of sensor screens whereas at project ID5827 it was used for the design of printable Thermoelectric modules contacts.

Autodesk fusion 360 was used at WUT (ID 5826) as a design and 3D modeling tool for 3D printing of substrates. Table 6 brings a list of all projects which accessed theorical provision from M1 to M30, the softwares used, and respective UoA.

Further details about the softwares offered by EMERGE host institutions can be found on deliverables D5.1 - Preparation of full modelling and simulation offer for the TAs and D5.2 - Comparison between different simulation and modelling programs used by different partners.

Table 6: List of softwares used for theorical access provision (TA1) from M1 to M30, and respective UoA.

Call/ Proposal ID	Proposal title	EMERGE Institution	Originally submitted to TA1	Software used	TA1 UoA
2nd Call 3829	Uniformity in visual appearance of individual cells in laminated OPV devices	JOR	Yes	Matlab	1

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2nd Call 3832	High-throughout exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films	FZJ	Yes	PFSim-Prost FZJ-DCFI	1
2nd Call 3833	High-throughout exploration of crystaline phase diagram space for the accelerated design of organic thin films	FZJ	Yes	PFSim-Prost FZJ-DCFI	1
3rd Call 4001	Formulating screen printing ink/paste application for resistive heater application	WUT	No	AutoCAD	1
4th Call 4625	Mass production of NFC tags printed on paper with additive techniques and at least 2 years lifetime, easy to recycle.	RISE	No	CAD (Adobe Illustrator)	1
4th Call 5682	Evaluation of scalability of 2D printing of magneto-rheological and magneto-electrical composites	RISE	No	CAD (Adobe Illustrator)	1.5
4th Call 5814	Screen-printed structures of alternating TiO2 and CeO2 layers used as an oxygen-sensing materials	RISE	No	CAD (Adobe Illustrator)	1.5
4th Call 5826	2D/3D CELL-PILs for tissue engineering	WUT	No	Autodesk Fusion 360	0.9
4th Call 5827	Manufacturing and Characterization of Flexible Thermoelectric Modules and associated electronics through printing techniques	RISE	No	CAD (Adobe Illustrator)	0.5

4. Expected Scientific Impact of Concluded Projects

The method developed on project 3829 leads to a minimization of the inhomogenities while keeping the efficiency losses of the LEH model on a low level. This improves the visual appearance of the active area where the module is visible resulting in a more visually pleasing look. Being able to adapt the appearance of Epishine's LEH modules to the existing, and often hard to change, design language of a variety of mass-produced wireless products enhances the adoption rate of LEH technology in general and Epishine's adoption

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rate in particular.

Besides that, the outcomes of this project can benefit the scientific society as the potential contribution of LEH modules for FLAPEP is to replace single-use batteries in battery-driven products with a substantially smaller energy storage and an LEH module, which charges the energy storage. This reduces the reliance on single-use batteries, reduces the amount of battery waste and reduces the ethical and environmental issues connected to sourcing materials for batteries. With the reduction of battery reliance through the implementation of LEH technology comes also a reduced environmental impact, e.g., expressed through an order of magnitude reduction in global warming potential (GWP) and ecotoxicity.

Professor Olga Wodo from University of Buffalo (USA), the user from projects 3832 and 3833, was significantly benefited from the opportunity to participate in the EMERGE call. The possibility to access trained professionals streamlined the analysis and acerated her research on the optimization of organic blends for organic photovoltaic cells.

Both projects hypothesized that using the full phase diagram for material screening would result in better design rules for material selection, especially for organic photovoltaics (OPV). Project 3832 focused on the exploration of amorphous multicomponent phase diagram space for the accelerated design of organic thin films while project 3833 focused on the crystalline phase diagram.

The main achievements of the projects were the generation of 245 ternary phase diagrams each for amorphous blends (ID 3832), and the generation of six libraries with 405 temperature-dependent phase diagrams each for crystalline binary blends (ID 3833). This data can benefit the scientific community, as it most likely will lead to a publication about the design rules for the organic blends.

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