



Open innovation platform for material modelling in organic electronics

MUSICODE addresses the Horizon 2020 Call number DT-NMBP-11-2020 “Open Innovation Platform for Materials Modelling” with the aim of creating a comprehensive modelling environment for materials design and processing, and device optimization in the Organic Electronics application domain. The platform integrates: modelling workflows spanning the micro-, meso- and macro-scales; graphical user interface tools for workflow design; a data management and execution framework with ontology-based semantic interoperability and plug-ins to Materials Modelling Marketplaces, the Open Translation Environment, and HPC infrastructures. Industry workflows for optimizing material properties and manufacturing will be demonstrated.

The challenge for modelling is to enable expeditious and accurate business decisions targeting high efficiency, performance and manufacturability while reducing errors, defects, resource waste, and performance variabilities.

But maintaining industrial competitiveness also requires efficient design, fast uptake of new materials, and smart adaptation of processing conditions.

This makes the challenge even more complex and ambitious given the sheer number of new candidate materials being discovered every year and the multitude of processing variations.

Nevertheless, this great challenge is also a great opportunity. Organic and Large Area Electronics (OLAE) do not share the same restrictions as their inorganic counterparts: candidate materials are unlimited; process

changes are not prohibitively expensive; there are less cross-contamination issues when changing materials; there are few compatibility issues; there are no prior-investment issues. Multi-scale modelling

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- University of Ioannina (Coordinator)
- Karlsruhe Institute of Technology
- University of Surrey
- Aristotle University of Thessaloniki
- Czech Technical University in Prague
- Fluxim AG
- TinniT Technologies GmbH
- Ansys
- ESTECO SPA
- Organic Electronic Technologies
- AIXTRON



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website:
musicode.eu



can be a guide through this largely unexplored terrain and become a decisive tool in propelling the OLAE industry's design capacity and productivity towards world leading applications and products.

This is the vision and objective of MUSICODE: to create an Open Innovation Platform for Materials Modelling and unleash the potential of OLAE. The project objectives are:

1. Develop novel validated multiscale modelling workflows for OLAE materials, processing, and devices;
2. Develop an ontology-based integrated modelling platform for workflow design, execution, data management;
3. Cooperate with EU stakeholders (European Materials Modelling Council, Marketplaces and High Performance Computing centers) for a complete customer offer.
4. Implementation of modelling workflows to optimize the manufacturing of organic photovoltaics (OPV) and organic light emitting diodes (OLED).

MUSICODE aims to create modelling workflows spanning the micro-to-macro (electronic-to-continuum) length scales and address specific problems related to the development and fabrication of OPV devices.

These include the effect of the material structure, photoactive blend composition, dopant concentration, and process parameters (e.g. nozzle shape, temperature, ink viscosity, printing speed, substrate treatment) on final material properties and device performance. The chosen physics models are run hierarchically with the output of one becoming the input for the next, returning results and key performance metrics back to the user.

Modelling scales include electronic and atomistic (UoI), mesoscale (KIT), continuum (TinniT), and device (Fluxim). To compile the modelling workflows, a novel workflow editor will be developed based on the Business Process Model and Notation (BPMN 2.0) standard and ESTECO Cardanit tool.



OET's OPV installations in an agricultural green house

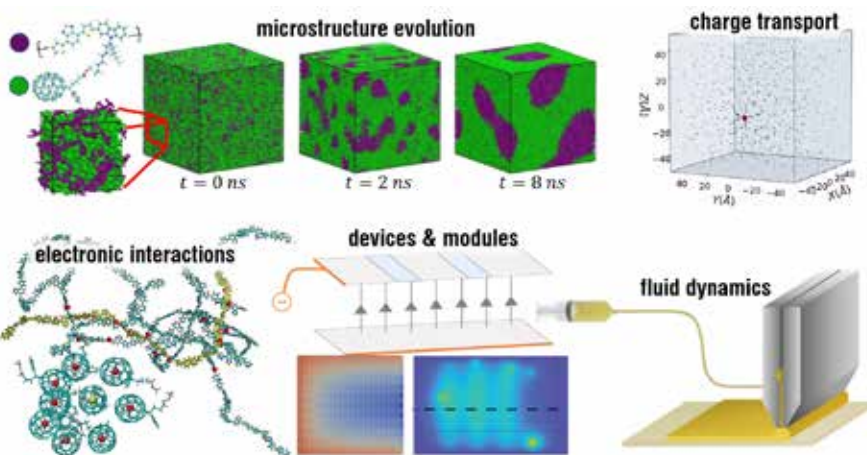


R2R pilot line to validate the modelling workflows

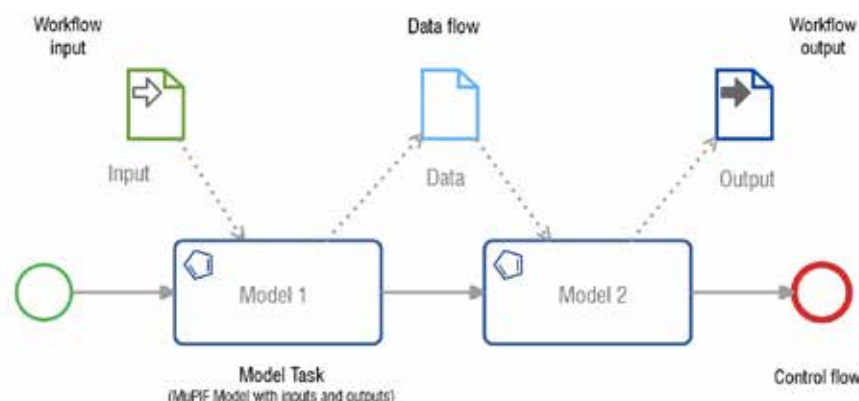
The workflows will be delivered to a novel interoperability layer (CVUT:MuPIF) for execution and then to an innovative data management system (Ansys:MI) for data population and traceability.

Careful validation is key to the successful implementation of modelling. MUSICODE models will be tested with extensive experimental fabrication and the characterization of materials and devices (AUF, USUR, Fluxim) and validated in real industrial pilot lines (OET, AIXTRON).

Our goal is for MUSICODE to become the central EU open innovation platform and repository for modelling, workflows, data, and metadata in Organic Electronics.



MUSICODE's multiscale modelling, from electrons to devices



ESTECO's novel workflow editor for multiscale modelling

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