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)

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Modelling of optimized OLAE devices

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Publishable summary

This document reports the work carried out in the Task 2.4 “Device and module modelling (M1 – M36)” under the WP2 “Development of multiscale modelling tools (M1 – M36)”. WP2 develops modelling tools from micro- to meso- and macroscale to simulate fabrication processes, material parameters and device performance of OE materials and devices. Task 2.4 focusses on opto-electronic simulations of thin film multi-layer device and large-area (including module) simulations. In collaboration with the partners, Fluxim adapted and extended its commercially available simulation tools Setfos and Laoss to improve the models and facilitate a satisfying user-experience.

This report shows the modelling work undertaken so far in Task 2.4. New models for devices to account absorption of photons and regeneration of charges in based on perovskite materials have been developed and demonstrated in multiple examples. Part of this work has been published in peer-reviewed journal.[1]–[3] Moreover, a robust fitting routine for transient photoluminescence experiments is developed that allows to quantify electrical material parameters of perovskite film from optical experiments. For OLEDs, a master equation model to simulate the exciton dynamics has been implemented in the commercial software Setfos. An example simulation shows the benefit of this new model for simulating physically meaningful, long-range transport and leakage into other layers. Moreover, a link between device and large-area/module simulations was introduced in the Laoss software (“Laoss – Setfos integration”). This link allows a user to analyze the effect of material or device parameters on the solar cell module performance. Finally, also large-area simulations are presented that demonstrate the capabilities of the tool to predict the optimal electrode layout or the ideal module configuration.