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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Publishable summary

This document outlines the progress achieved in modelling and validation of material related charge carrier mobilities obtained for ternary donor-acceptor molecular systems for OPVs. It is a natural continuation of the tasks set in WP6 of the Musicode project. It builds up on already submitted deliverables such as D6.1 (OET, M24) “Lab and large scale OLAE devices with doped organic semiconductors by printing”, D6.2 (OET, M30) “Lab and large scale OPV devices with ternary photoactive nanolayers”, and D6.3 (USUR, M36) “Report on dopants in OE material mobility (modelling and validation)”.

The report includes results based on modelling of ternary donor/acceptor molecular systems for OPVs, specifically PCDTBT/IDIC/ICBA, which was accomplished by using thermodynamic energies (interface and Gibbs total) of the molecules studied in WP2. Furthermore, PFM simulations as a function of temperature and boundary conditions were performed to explore the possible microstructures and phase-space of ternary combinations. Backfilling to atomistic detail and molecular, microelectrostatics, and Monte Carlo modelling revealed intricate energetic changes at the material interfaces as well as the carrier mobilities of the ternary blend. Optical modeling based on SE data from single layers and binary or ternary blends was also used to simulate the optical limit of a device where one can vary the thickness of the active layer as well as the mixing ratio of the components for the binary blend.

Moreover, small- and large-area OPV devices were fabricated and characterized by experimental partners. Herein, small-area OPVs based on the ternary blend of PM6:D18:L8BO were fabricated, and their performance was evaluated at different light intensities reaching a PCE of above 17.5%. Stability studies were also carried out. Additionally, for large-are OPV devices the impact of different A1:A2 ratios in the ternary blend PBDB-T:BTP-12:$PC_{60}BM$ was studied. Numerous samples of both single carrier and OPV devices were fabricated, and the mobility of the blend extracted to validate the best performance of organic solar cells.