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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Report on dopants in OE material mobility (modelling and validation)

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Publishable summary

This document outlines the progress achieved in modelling and analysis of the doping effect in OE materials and devices. Special attention is given to the influence of the doping on the physical properties of OE materials, such as alteration of the charge carrier mobility. The modelling data generated by UOI and FLUXIM is based on the experimental input provided by AUTH, OET, and USUR. This report is a continuation of the activities reported in D6.1. Results included in this document show the successful fabrication, characterisation, and modeling of PCDTBT- and PBDB-T- based HOD doped (and not) with F4TCNQ. Herein, trends of measured JV key figures from pristine and doped devices could be reproduced by device simulation. Additionally, optical, and structural characterization of doped PBDB-T and PBDB-T:BTP-12 layers were carried out. Ultimately, hole mobility values from PCDTBT and PBDB-T were extracted. Furthermore, the effect of using F4TCNQ as a dopant material for PBDB-T:BTP-12-based OPVs was studied showing an OPV device performance improvement with the increase in dopant concentration up to a certain threshold. Modelling results of carrier mobility as a function of doping concentration are shown for the PCDTBT:F4TCNQ and IDIC:BV systems using multiscale charge transport simulations.