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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Templated modelling use case workflows on dopants in OE materials

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Publishable summary

In Organic Electronic (OE) devices, one crucial property is the ability of the organic material constituents to conduct, i.e., to transport electron and/or holes from one molecule to the next and thus from one device terminal to the other. This charge transport ability is quantified by the carrier mobility. Given their organic nature, charge transport occurs through thermally activated diabatic hops between neighboring molecules. A method to tune and optimize this process (amongst others) is the addition of suitable dopants, i.e., small organic molecule additives, either n- or p-type, in small concentrations.

Charge transport is a complex process, stochastic in nature, affected by the molecular microstructure, the molecular energy levels, as well as the inter-molecular interactions. Its modelling requires multiscale modelling, involving electronic calculations (Density Functional Theory) for molecular energies and interactions, atomistic simulations (Molecular Dynamics) for the microstructure in molecular ensembles, and mesoscopic simulations (microelectrostatics and kinetic Monte Carlo) for transition rates and charge hopping. Post processing of the simulation results yields the carrier mobility as a function of temperature and applied electric field, which is then fitted to a standard Gaussian Disorder Model (GDM) functional for OE mobility so that it can be directly used in continuum device models.

To address the high complexity of doing multiscale modelling with endless material combination (OE molecule + dopant), MUSICODE standardized and templated a modelling workflow that allows the user to just pick the molecule combinations and concentrations of interest from the Data Management System (DMS), and upon execution directly get the GDM-fitted mobility function. This document describes the methodologies and the templated modelling workflow created in the Workflow Editor, provides a manual for API generation (targeted to expert users) and for workflow execution (targeted to non-expert users), and ends with some practical examples and results.