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

A crucial property of active organic electronic molecules is charge transport, i.e., transport of electrons and/or holes. Carrier mobility quantifies the ability of these molecules to conduct and has a high impact on the overall performance of the OE devices. Given their organic nature, charge transport occurs through thermally activated diabatic hops from one molecule or one monomer to the another. This is a complex process, affected by the molecular microstructure, the molecular energy levels, as well as the inter-molecular interactions. The process itself is complex, being stochastic in nature. MUSICODE addresses this with a multiscale modelling scheme involving electronic calculations (Density Functional Theory) for molecular energies and interactions, atomistic simulations (Molecular Dynamics) for the microstructure in molecular ensembles, and mesoscopic simulations (kinetic Monte Carlo) for 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 standard functionals of OE mobility so that it can be used in continuum device models. This document describes the methodologies and results obtained for several molecules of interest up to M23 of the project. The modelling workflows created here will be templated in the Workflow Editor so that users can automatically execute them for a variety of different molecules and molecular ensembles.