



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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### Specifications of the material modelling tools

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## 1. Executive summary

The MUSICODE platform enables interoperable multiscale simulations on organic electronic materials, devices, and processes. Such multiscale modelling workflows are built by a hierarchical assembly of specific and well-defined modelling tasks. These modelling tasks operate at different scales, they require and produce different data, and have different validity ranges. This document highlights the different modelling tools and modelling tasks that will be assembled within the MUSICODE workflows for Organic Electronics, and lays down the detailed specifications for data, solvers, validity ranges, convergence criteria, approximations, etc. This document will serve as a guide for all modelling activities in the MUSICODE project, including simulation data storage, transfer, documentation, metadata, OLAE ontology buildup, model API construction, etc.