



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

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, each one operating at a different length scale. The multiscale character of these modelling workflows stems from the fact that the simulation results of one model at a lower length scale (i.e., at finer description detail, e.g., atomistic) are used to parametrize another model at a higher length scale (i.e., coarser description detail, e.g., mesoscopic). This process is termed “forward mapping”. MUSICODE has identified a total of 7 such mappings needed to construct a full modelling capability for organic electronics. These start from electronic scale models using density functional theory methods and ending up to continuum scale models using computational fluid dynamics. This document describes each mapping, the scales involved, the need for it, the methodology used, the materials and systems applied to, and the results obtained up to M17 of the project.