



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 integrates physical models and solvers covering all length scales, i.e., electronic, atomistic, mesoscopic and continuum. Their hierarchical execution targets the simulation of different complex phenomena and processes, such as charge transport in organic semiconductors, thermodynamics of microstructure evolution, vacuum deposition of molecules, roll-to-roll processing of organic films, and more. To create a seamless and user-friendly environment even for the non-expert user, MUSICODE integrates a data management system (DMS) holding all data and workflows, a workflow editor (WE) for compiling multiscale executable scripts linking models to data, and an execution layer (MuPIF) that manages workflows, models and data, their execution in HPC facilities, and the communication to/from the DMS.

This deliverable “Modelling Protocols & Documentation” aims to serve as a comprehensive manual for developers engaging with the MUSICODE platform, i.e., for expert modelers and software/solver providers. Specifically, for each solver it documents the data requirements for execution (solver I/O) and the integration methodology of this solver in the platform, i.e., definition of model metadata and creation of model API (wrapper), so that it efficiently utilizes the MUSICODE ontological data containers, and in turn, is itself efficiently handled by the WE and MuPIF. By documenting these processes for several models in different scales and physics, this deliverable essentially becomes the complete manual for inserting a new model (i.e., solver) in the platform, and as such it will be utilized (pending a final update and polishing at M48) after the end of the project.