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 user case workflows on ternary OE materials

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Publishable summary

This deliverable describes the development of a streamlined workflow template that allows a systematic study of ternary organic material formulations. This study bridges two distinct domains, the mesoscale where thermodynamic based calculations via the Phase Field Method simulate and predict the microstructures attainable by the organic material combinations, while atomistic methods based on molecular dynamics, density functional theory and kinetic Monte Carlo re-introduce the atomistic detail in the predicted microstructure and go on to predict important electronic properties that are crucial to the materials performance in a device. By leveraging MUSIOCDE's Workflow Editor for task visualization and Python script generation, data integration, and MuPIF's smooth execution capabilities, this workflow enables a cohesive, end-to-end modeling experience across the different scales.