



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 Gas Phase Processing in OE Materials

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## Publishable summary

This deliverable describes the development of streamlined workflow templates that allow a systematic study of gas phase deposition of organic molecules on a substrate. This study bridges two distinct domains, the macroscale where computational fluid dynamics simulate the gas flow lines in the reactor and through the showerhead of an OVPD system, while atomistic methods based on molecular dynamics simulate the molecular deposition in atomistic detail, following two distinct paths: the forward one, where multiple parallel stochastic depositions (variable angles and speeds) are used to quantify a sticking coefficient to be used as input in the CFD simulations, or the output of CFD (angles and speeds) are used as input in multiple sequential MD simulations of film growth.