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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Glossary

AFM	Atomic Force Microscopy
DOS	Density of States
EMT	Effective medium theory
ex-situ	outside fabrication chamber
GIWAXS	Glazing-Incidence Wide-Angle X-ray Scattering
in-line	real-time on R2R pilot line
in-situ	within fabrication chamber
IR-Vis-UV	Infrared-Visible-Ultraviolat
KPFM	Kelvin Probe Force Microscopy
PL	Photoluminescence
R2R	roll-to-roll printing
RS	Raman spectroscopy
SE	Spectroscopic ellipsometry
SOR	Successive Over-Relaxation
VASE	Variable-angle SE
XRR	X-Ray Reflectance

Contents

Publishable summary

The deliverable reports the MUSICODE activities within WP3 Task 3.2 regarding optical and structural characterization for model validation, coupled with the corresponding modelling activities in WP2 which were set to produce quantitative estimates on measurable physical quantities and enable direct comparison to experiments. Specifically, it reports measurements on organic electronic material layers, both pure and blended, fabricated by spin coating or printing. The experimental techniques include spectroscopic ellipsometry, Raman spectroscopy, photoluminescence, atomic force microscopy, x-ray reflectance, and thermogravimetric- and differential scanning calorimetry analysis. The models to be validated include atomistic models utilizing the molecular dynamics technique and micro-electrostatics calculating self-consistently polarization screening effects. The physical quantities to be used for the model validation, i.e., measured experimentally and estimated theoretically, include the mass density, the glass transition temperature, and the real part of the (static) infrared dielectric constant. The comparison shows excellent scaling and qualitative agreement between modelling and experimental results, in some cases reaching very good quantitative agreement. The results reported here show the status of characterization and model validation up to M29. The corresponding tasks in WP2 and WP3 are running up to M36 with more characterization and model validation activities already in development.