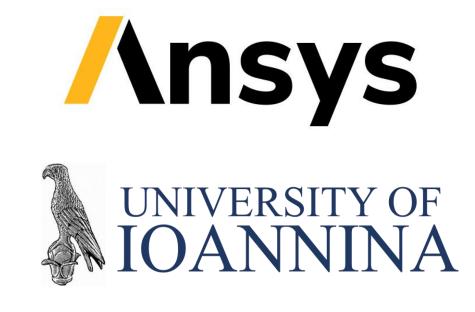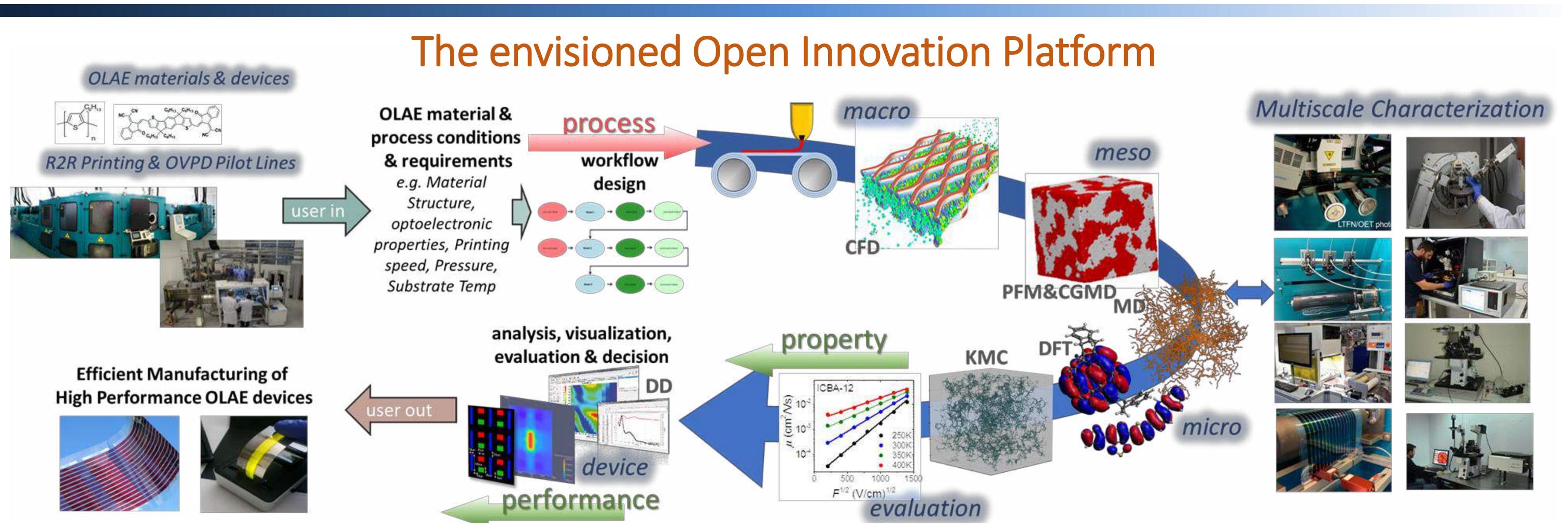# MUSICODE Open Innovation Platform For Materials Modelling

musicode

MUSICODE has the ambitious goal of developing an Open Innovation Materials Modelling Platform to expedite accurate and knowledgeable business decisions on materials design and manufacturing process optimization. The platform offers multiscale modelling capabilities, workflow editing and execution, data management and HPC support, being demonstrated in the Organics and Large Area Electronics application domain in four industrial use cases.

Ansys

UNIVERSITY OF IOANNINA

The envisioned Open Innovation Platform

OLAE materials & devices

R2R Printing & OVPD Pilot Lines

user in

OLAE material & process conditions & requirements
e.g. Material Structure, optoelectronic properties, Printing speed, Pressure, Substrate Temp

process workflow design

macro
CFD

meso
PFM&CGMD
MD

Multiscale Characterization

Efficient Manufacturing of High Performance OLAE devices

user out

analysis, visualization, evaluation & decision
DD

device
performance

property

KMC
DFT

micro

evaluation

	use cases	user interface	modelling	validation
	OET, AIXTRON	ČVUT, ESTECO, Ansys	FLUXiM, UNIVERSITY OF IOANNINA, KIT, TiNNiT	ltfn, ARISTOTLE UNIVERSITY OF THESSALONIKI, UNIVERSITY OF SURREY
	• new material formulations	• integrated data management	• ontology-based interoperability	• multiscale characterization
	• solution-based processing	• workflow design, optimization	• electronic to continuum models	• material model validation
	• gas-phase transport	• linked to Marketplaces	• process-property relations	• industry-accepted protocols
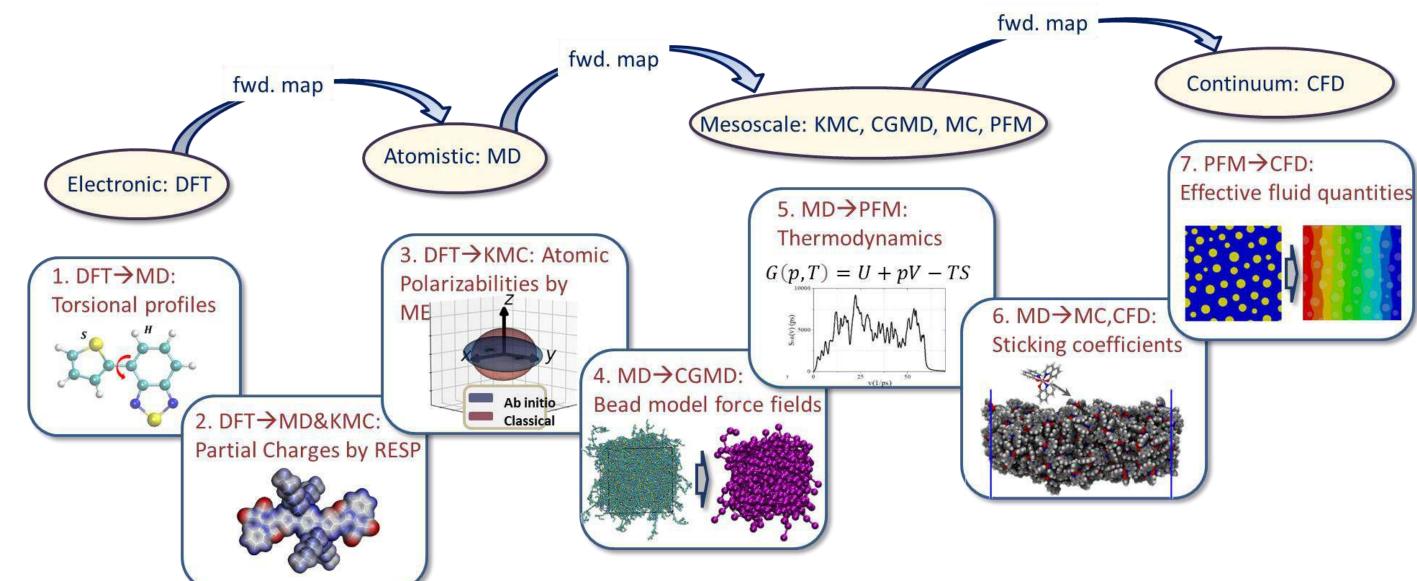
The offered modelling capabilities
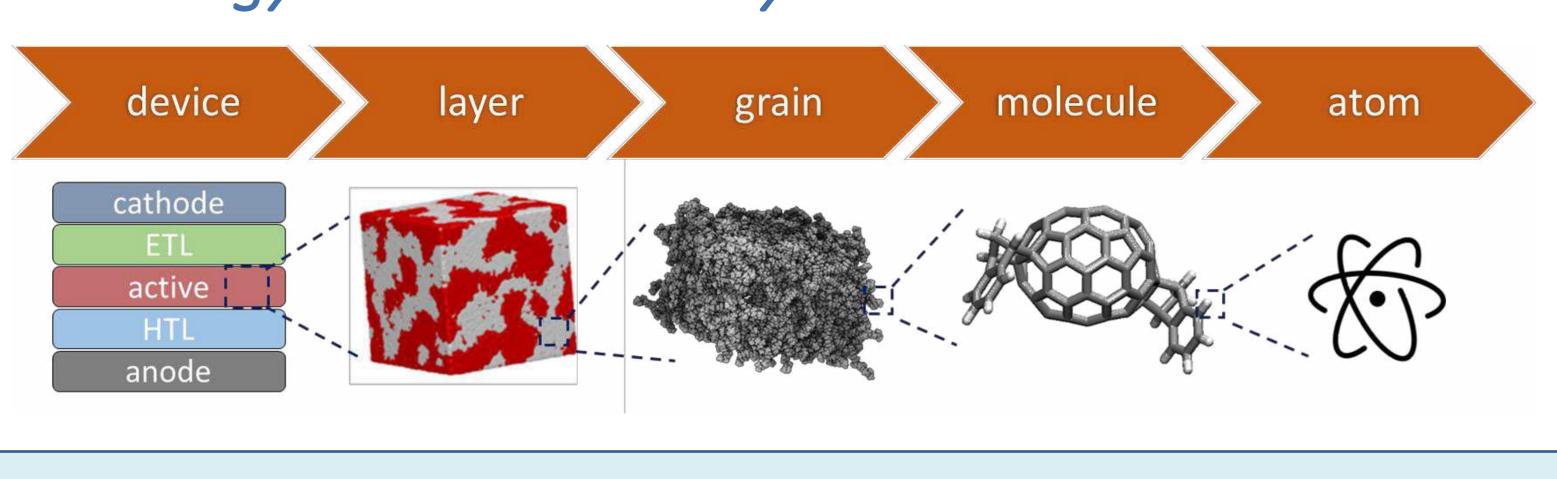
Multiscale modelling and simulations

microstructure evolution

$t = 0\ ns$ $t = 2\ ns$ $t = 8\ ns$

charge transport

electronic interactions

devices & modules

fluid dynamics
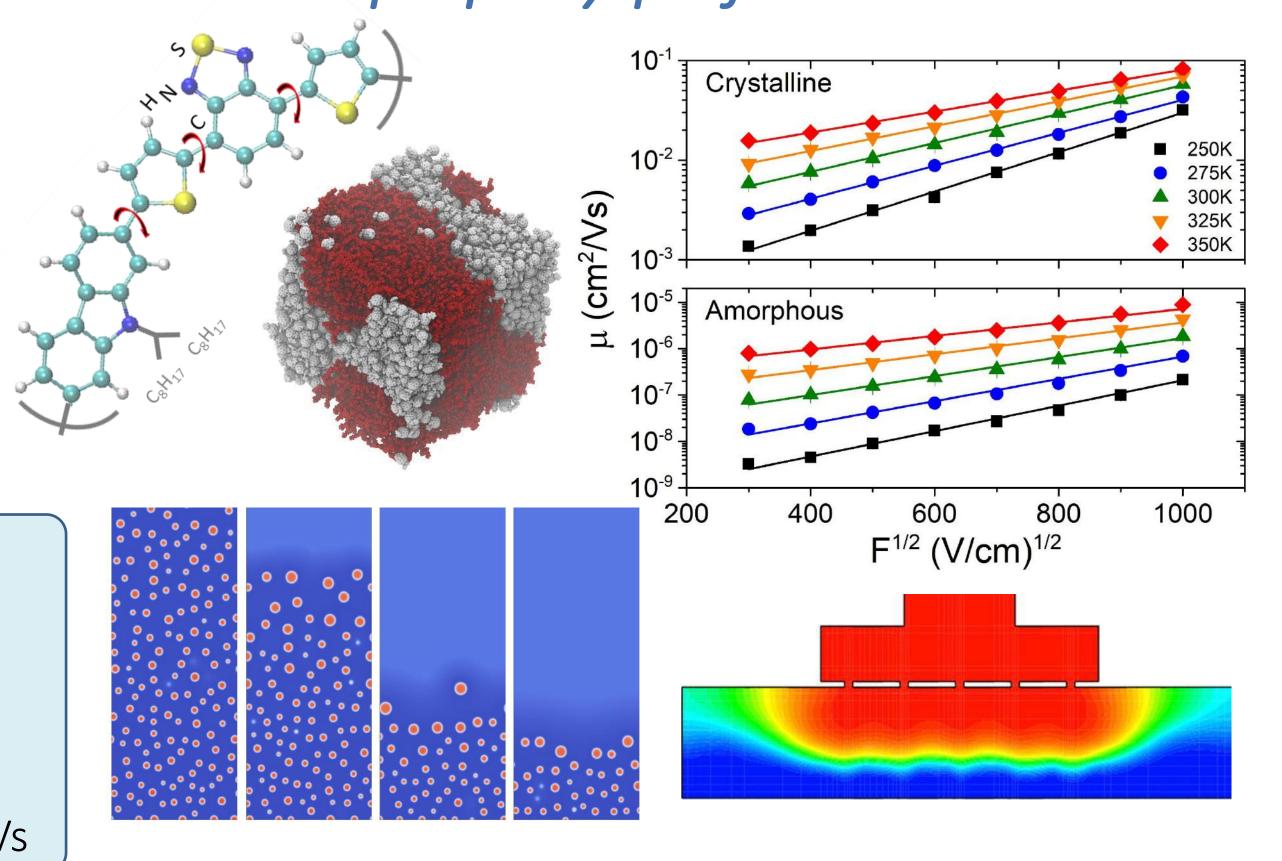
Forward and backward mappings between scales

fwd. map   fwd. map   fwd. map

Electronic: DFT → Atomistic: MD → Mesoscale: KMC, CGMD, MC, PFM → Continuum: CFD

1. DFT→MD: Torsional profiles

2. DFT→MD&KMC: Partial Charges by RESP

3. DFT→KMC: Atomic Polarizabilities by ME

4. MD→CGMD: Bead model force fields

5. MD→PFM: Thermodynamics $G(p,T) = U + pV - TS$

6. MD→MC,CFD: Sticking coefficients

7. PFM→CFD: Effective fluid quantities

Ontology and semantically linked data structures

device → layer → grain → molecule → atom

cathode
ETL
active
HTL
anode

Process-structure-property-performance relations

Crystalline

■ 250K	▲ 300K
● 275K	▼ 325K
	◆ 350K

Amorphous

μ (cm^2/Vs)

$F^{1/2}$ (V/cm)$^{1/2}$

The industrial use cases to be demonstrated:

1. Effect of n/p-type dopants into OPV and OLED active materials
2. Optimization of ternary donor/acceptor molecular systems for OPVs
3. Gas-phase processing and optimization of vapor deposition parameters for OLEDs
4. Solution-based processing and optimization of slot die printing parameters for OPVs