D2.1 First version of the CORNET database

Date: 03-07-2018

Multiscale Modelling and Characterization to Optimize the Manufacturing Processes of Organic Electronics Materials and Devices

(CORNET)

Grand Agreement: 760949

Horizon 2020
European Union funding
for Research & Innovation

This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call

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Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission Service	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (excluding the Commission Services)	

Deliverable Report			
Deliverable No.	D2.1		
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Change Management			
Version	Date	Author(s)	Comments
0.1	03-2018 - 06.2018	GRANTA	Schema and structure development requirements (series of web meetings)
0.2	22.06.2018	GRANTA	Demonstration for partners
0.3	25.06.2018	GRANTA	Release of database to partners (partners have read/write access)
0.4	30.06.2018	GRANTA	Summary of work done for partners (presentation, report)

[1] Please use the same as in the DoA. **PU** =Public, fully open, e.g. web. **CO** = Confidential, restricted under conditions set out in Model Grant Agreement. **CI** =Classified, information as referred to in Commission Decision 2001/844/EC.

[2] Please Use the same as in the DoA. **R:**Document, report (excluding the periodic and final reports). **DEM**:Demonstrator, pilot, prototype, plan designs. **DEC:** Websites, patents filing, press & media actions, videos, etc. **OTHER:** Software, technical diagram, etc. **ORDP**: Open Research Data Plan.

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	University of Ioannina	Greece
	Centre National de la Recherche Scientifique	France
	Fluxim	Switzerland
	Aixtron SE (AIXTRON)	Germany
	National Physical Laboratory	UK
	Organic Electronic Technologies Private Company IKE (OET)	Greece
	Centro Ricerche FIAT SCPA (CRF)	Italy
	Granta Design	UK
	Hellenic Organic & Printed Electronics Association	Greece

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Acronym Summary

AFM	AFM: Atomic Force Microscopy
BIPV	BIPV: Building Integrated PVs
CA	CA: Consortia Agreement
Can	CAn: Contact Angle
CAE	CAE: Computer Aided Engineering
CELIV	CELIV: Charge Extraction Linearly Increasing Volt
CGMD	CGMD: Coarse grained molecular dynamics
CV	CV: Capacitance Voltage
CVD	CVD: Chemical Vapor Deposition
CVo	CVo: Cyclic Voltammetry
DFT	DFT: Density Functional Theory
DMP	DMP: Data Management Plan
EMCC	EMCC: European Materials Characterization Council
EMMC	EMMC: European Materials Modelling Council
FAIR	FAIR: Finable, Accessible, Interoperable, Re-usable
FDTD	FDTD: Finite-difference Time-domain
FE	FE: Finite Element
GB	GB: Giga bytes
GIWAXS	GIWAXS: Grazing-incid. wide-angle x-ray Scatter.
HTL	HTL: Hole Transport Layer
KMC	KMC: Kinetic Monte Carlo
KPI	KPI: Key Performance Indicator
LBIC	LBIC: Light Beam Induced Current
LUMO	LUMO: Lowest Unoccupied Molecular Orbital
MB	MB: Mega bytes
MC	MC: Monte Carlo
MD	MD: Molecular Dynamics
MODA	MODA: Modelling Data elements
NI	NI: NanoIndentation
NIST	NIST: National Instit.of Standards & Technology
OLED	OLED: Organic Light Emitting Diodes
OPV	OPV: Organic PhotoVoltaics
ORDP	Open Research Data Pilot
OTFT	OTFT: Organic Thin Film Transistor
OVPD	OVPD: Organic Vapour Phase Deposition
PCE	PCE: Power Conversion Efficiency
PL	PL: Photoluminescence
PoC	PoC: Proof of Concept
PPV	PPV: Perovskite PhotoVoltaics
PVD	PVD: Physical Vapour Deposition
R2R	R2R: Roll-to-Roll
RFID	RFID: Radio-frequency identification
RS	RS: Raman Spectroscopy
S2S	S2S: Sheet-to-Sheet
SE	SE: Spectroscopic Ellipsometry

SEM	SEM: Scanning Electron Microscopy
SNOM	SNOM: Scanning Near field Optical Microscopy
TB	TB: Tera bytes
TEM	TEM: Transmission Electron Microscopy
UPS	UPS: Ultraviolet Photoelectron Spectroscopy
VAMAS	VAMAS: Versailles Project on Adv. Mat. & Stand.
VASP	VASP: Vienna Ab-initio Simulation Package
VPN	VPN: Virtual private network
WP	WP: Work Package
WVTR	WVTR: Water Vapor Transmission
XPS	XPS: X-ray Photoelectron Spectroscopy
XRD	XRD / XRR: X-Ray Diffraction / Reflection

CONTENTS

1.0 INTRODUCTION

CORNET is an ambitious project submitted to the H2020 Call NMBP-07-2017, that will develop a unique EU Open Innovation Environment (OIE) covering the triangle of manufacturing, modeling and experimentation in order to optimize the Organic/Large Area Electronic (OE) materials, materials' behaviour and nano-devices (OPVs, PPVs, OLEDs) manufacturing processes. This will be achieved by linking the nanostructure features with the macroscopic functionality through multiscale (nano to macro) characterization and modeling. This will strongly impact the fast and reliable development of new materials, devices and will enable control of the related production processes (R2R printing and gas transport (OVPD)) to fabricate tailored OE devices and systems to demonstrate industrial applications (e.g. automotive, greenhouses).

Partners include: Aristotle University of Thessaloniki (Coordinator), Nanotechnology Lab LTFN, National Physical Laboratory UK, University of Surrey, Organic Electronic Technologies OET, Centro Ricerche Fiat, University of Ioannina, Centre National de la Recerche Scientifique CNRS, Granta Design, Fluxim, Hellenic Organic and Printed Electronics Association HOPE-A, AIXTRON.

The goal of this deliverable is to develop a sustainable database to host reference material data for the wider Organic Electronics ecosystem (academia, supply chain members across various platfroms and end-uses). The database has been implemented using the GRANTA MI materials information management system. This system has been developed over 15+ years to host materials information for manufacturing organizations using materials from classes such as metals, advanced polymer composites, ceramics, biological, etc., in domains such as aeorspace, automotive electronics, biomedical, energy, consumer goods, transport, among others.

2.0 CORNET Database Implementation, Alpha Version

There are three sources of data generated/collected in the CORNET project:

1. Modelling and simulation data produced by modelling software
2. Experimental data produced by machines and sensors
3. Device performance KPI's, which may be a combination of measured/actual and modelled/theorectical data

Table 2.1 summarizes partner capability in terms of characterization, modelling, and manufacturing, and specific methods/codes which are in themselves sources of data.

TABLE 2.1 Partner characterization capabilities relevant to the CORNET project

Partner	Characterization Tools	Modelling Approaches	Manufacturing
AUTh	SE, RS, PL, AFM, XRR, XRD, XPS, WVTR, CA, NI, SEM, TEM, Electrical, Nanoindentation	DFT, models for optical & optical engineering, electrical, mechanical	R2R & S2S printing pilot lines, OVPD pilot line for fabrication of OPV, PPV, OLED
USUR	Optical, PL, AFM, SEM, TEM, CA, Solar Sim. EQE, Electrical	SILVACO, COMSOL, charge transport, optical device	Fabrication OPV, PPV, OLED
UOI	SEM, TEM, Reflectance	MD, Mesoscopic, Charge transport	Computational modelling cluster
NPL	AFM, LBIC, PL, RS, WVTR, Stability measurements, metrology	2D Finite Element Device mod. charge transp. simulation	Stability, defects, modelling/simulation, protocols & validation, standardization
CNRS	SE, AFM, etc.	Compact Modelling	Compact modelling for devices
Fluxim	Electrical characterization: CV, TEL, Impedance Spectrosc, CELIV	Electro-optical device stack and large area simulation	Simulation tools for OPVs, OLEDs, test meas. of electrical properties
OET	Stability measurements, Solar simulator, In-line optical metrology	Modelling of SE, RS spectra	R2R fabrication of OPV, PPV, OLEDs by unique pilot lines. optical metrology
Aixtron	Electrical characterization	OLED process software	OVPD systems, process for OLEDs
CRF	SEM, AFM, Profilometry	Modelling for materials & stability in real conditions	Industrial testing of components and surfaces for automotive applications

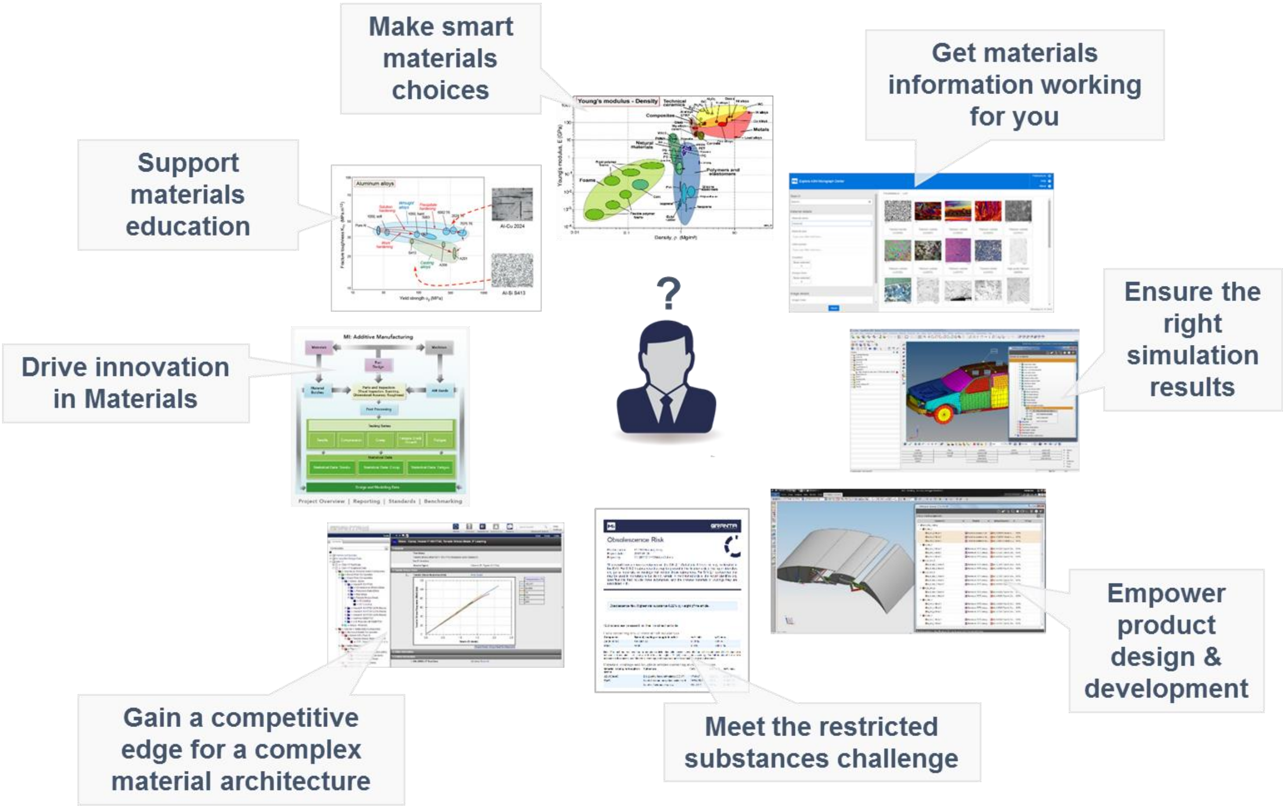

Figure 1.1 Use cases for managed materials information and data

Figure 1.1 illustrates various design decisions which materials and process information gleaned from characterization methods readily supports. The representative tasks include early design decisions such as material selection, to structured data required for detailed finite element design. Characterization with appropriate meta-data (or pedigree), data quality assurance and associated measure of uncertainty enable confidence in decision-making and reduces design iteration failure. When characterization is managed in a centralized database system, the savings are extended to elimination of lost test data, reduced time engineers/scientists spend searching for data/information, and reduced time spent rolling-up and analyzing data.[3]

[3] S Warde, R Painter, D Williams, A Fairfull, W Marsden, 2012, The Business Case for Materials Information Technology, Granta Design.

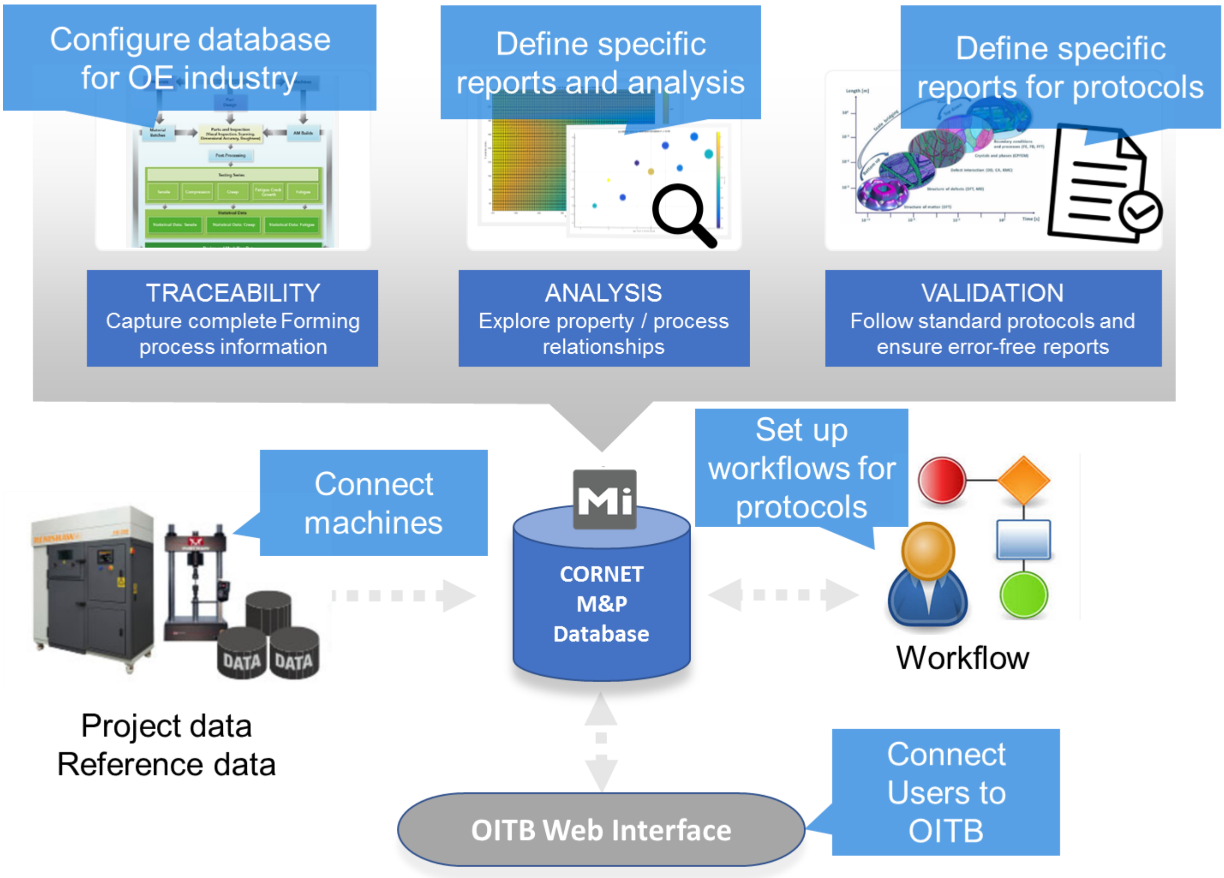

Figure 1.2 Illustratration of the OIE Materials Database system used in the CORNET project

Figure 1.2 illustrates the main components of the manterials information management system (GRANTA MI) implemented for the CORNET project: i) relational database which supports full traceability by creating meaningful links between database tables; ii) underpinning the database is a schema specific to the material (e.g. metals), processing (e.g. additive manufacturing) domain, and sector (e.g. OE); iii) import capability from machines and other reference databases; iv) analysis tools for exploring structure/property/process/performance relationships; v) custom reporting for qualification, validation, sustainability analysis, etc.; vii) workflow for tracking data as it is imported, stored, analyzed, reported against, sign-off and quality control, exported for use in specific design environment tools. The database will have a live link from the OIE Web Interface.

Implementation

All CORNET partners participated in weekly webex meetings during the period of March to June 2018, to structure the schema, record views, tables for the database, and to collect use cases for the OE industry, led by Materials Information Management Consultants from Granta Design. A schema will contain several tables detailing materials, process, part pedigree, characterization data (physical and virtual), which can add up to hundreds of attributes (often totalling over 1000 attributes for a given material domain for a specific sector).

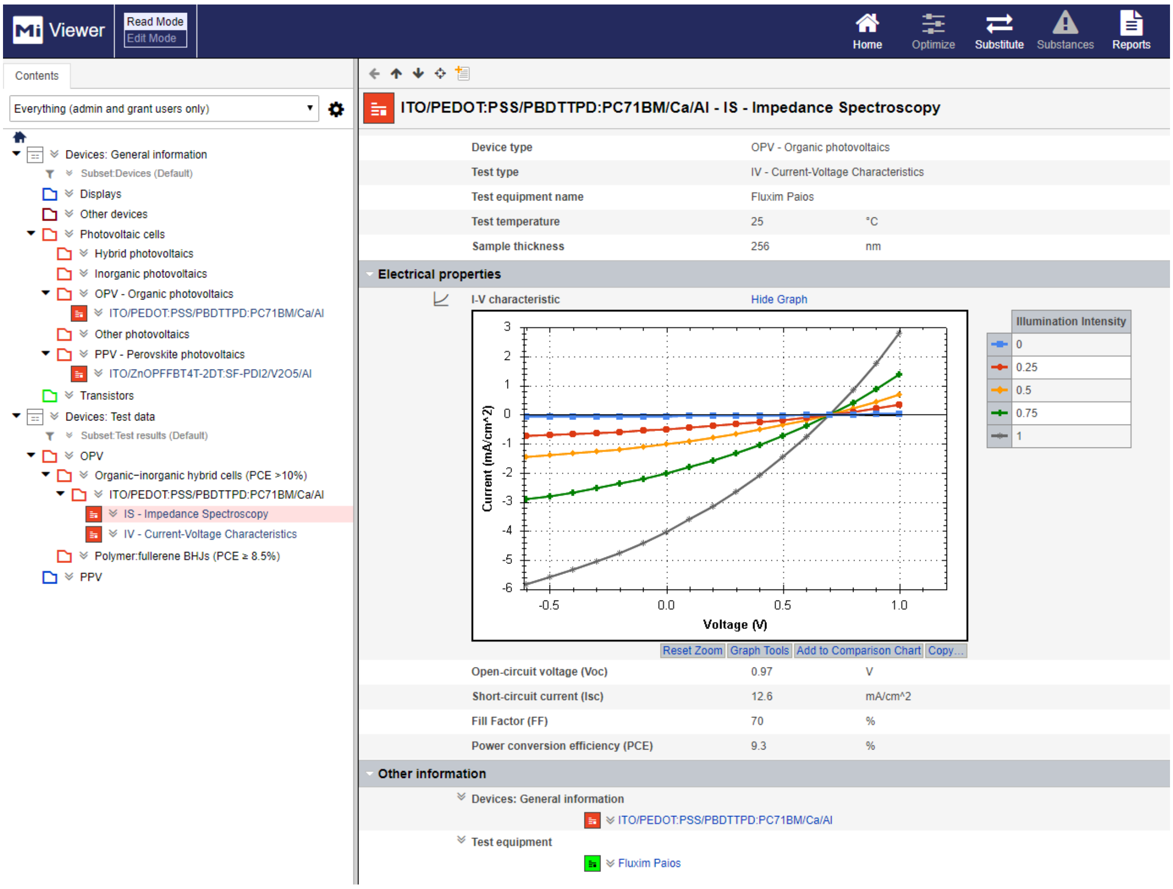

Figure 2.1 CORNET device record example demonstrating graphical data and links between tables

Figure 2.1 shows a screen shot of a device table and test record, demonstrating the control of functional data within the database and links between tables for traceability. This view was designed with the cooperation of partners for the OE industry. Figure 2.2 shows a screen shot of the homepage for the project database, enabling filtering on devices, layers and materials.

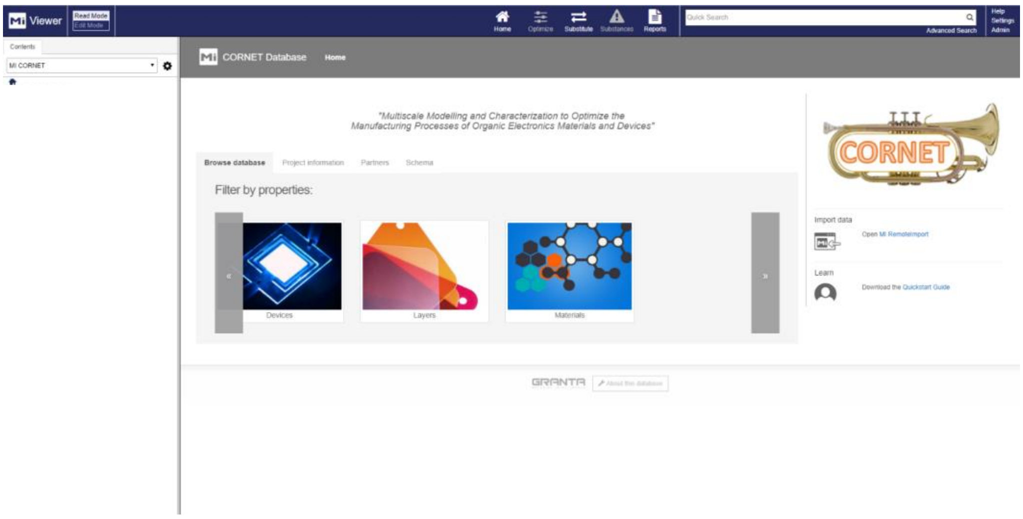

Figure 2.2 CORNET project database homepage

Next Steps

D2.1 represents the initiation of work to develop the CORNET database in preparation for public release at the end of the project. The following steps outline the work to release the database at the end of the project:

1. Database requirements survey (Months 1-6):
Specifications with partners
Schema development for characterization methodology collection
Storage strategy for measurement, modelling output

2. Database infrastructure development (Months 1-30):
Data models for multi-technique characterization
Metadata to support protocols
Performance for wider industry access

3. Database population (Months 1-36):
Characterization data population and protocols development
Development of reports to support the OE use cases