Materials Data in Electrical Device Design

Andrew Miller, Prof. David Cebon, Jean-Marc Lucatelli

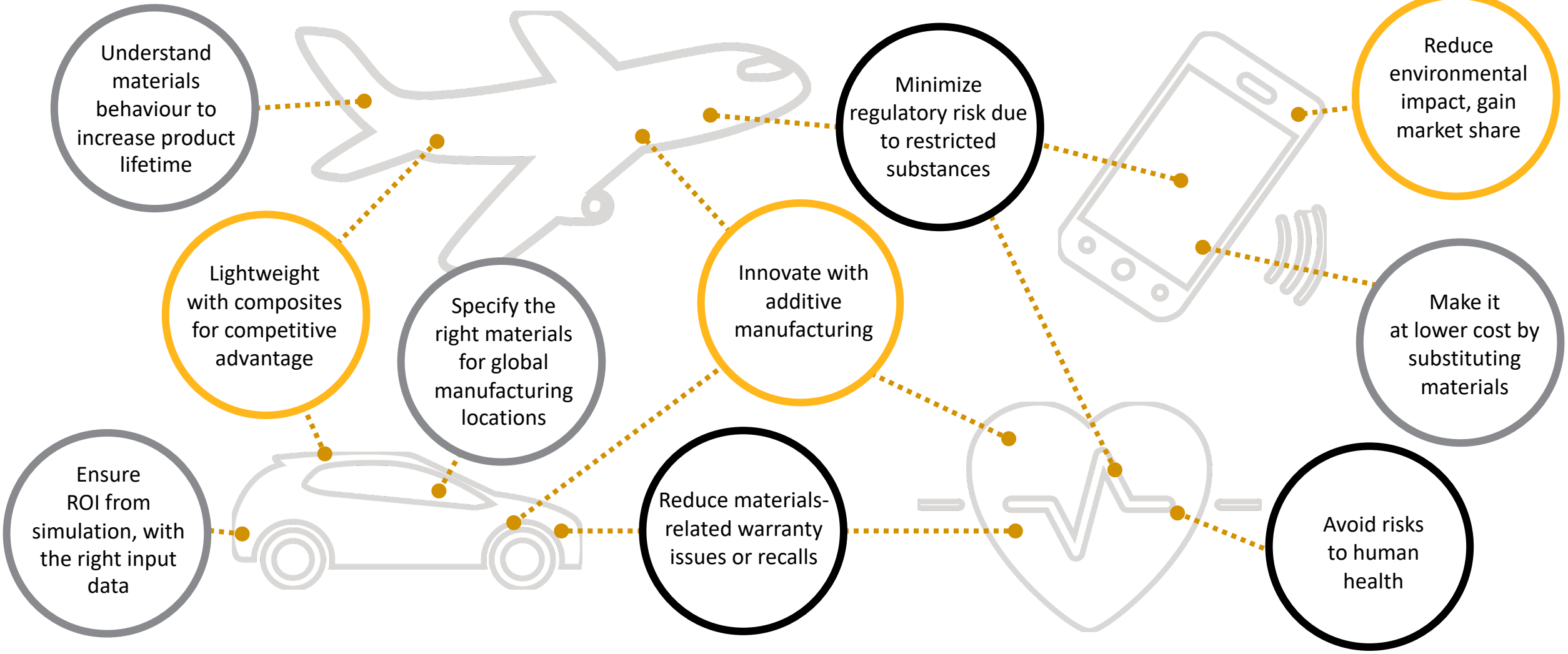
Ansys Granta, Cambridge, UK

Materials Data in Electrical Device Design

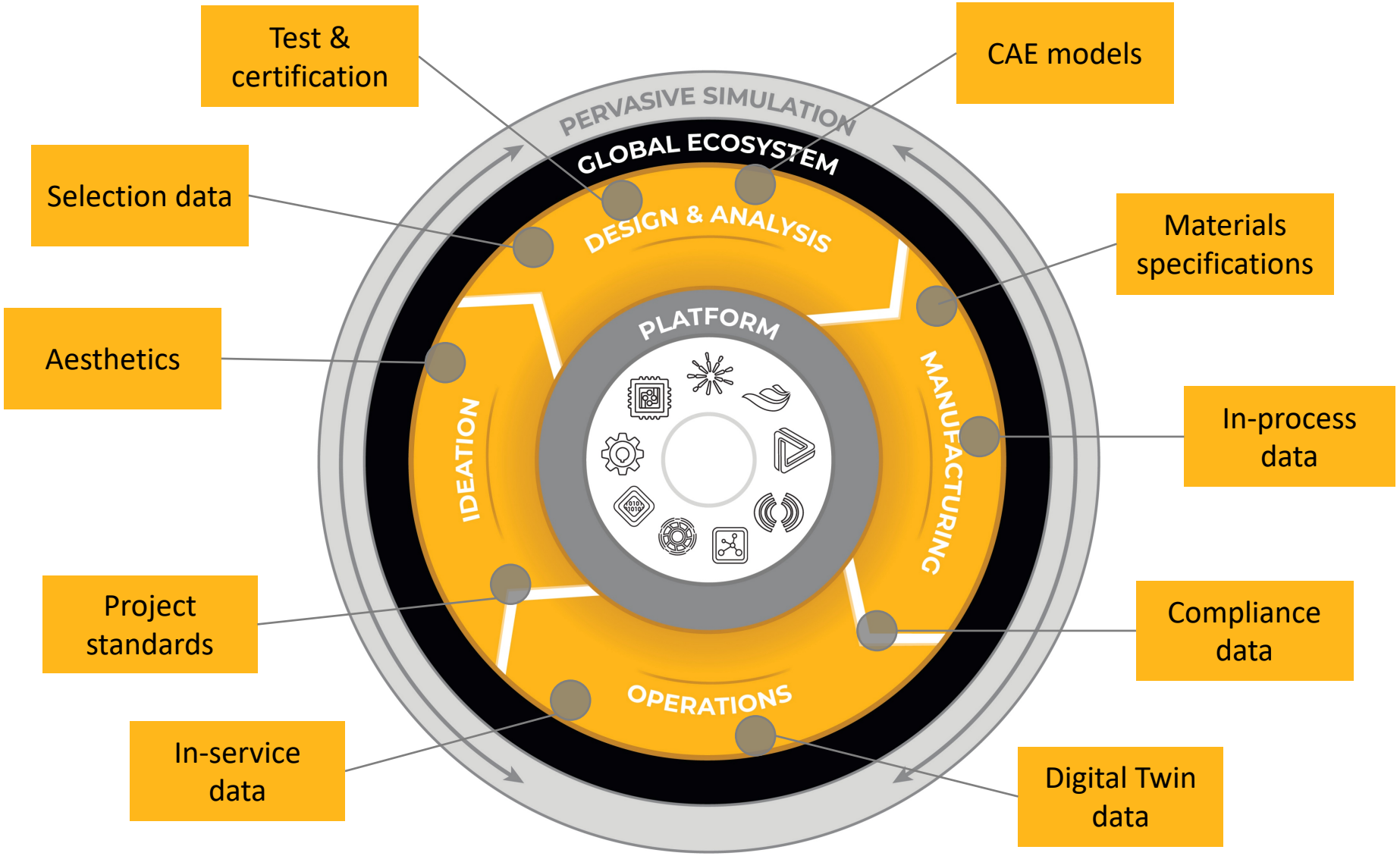
- The Importance of Materials & Materials Data
- Materials Data Management
- Integrated Computational Materials Engineering (ICME)
- Case Study: CORNET Project & Organic Electronics

Why materials information matters

Growth | Profit | Risk



Materials information throughout the product lifecycle



Test & certification

CAE models

Selection data

Materials specifications

Aesthetics

In-process data

Project standards

Compliance data

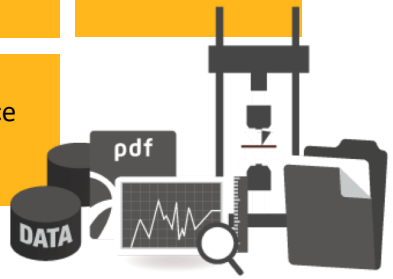
In-service data

Digital Twin data

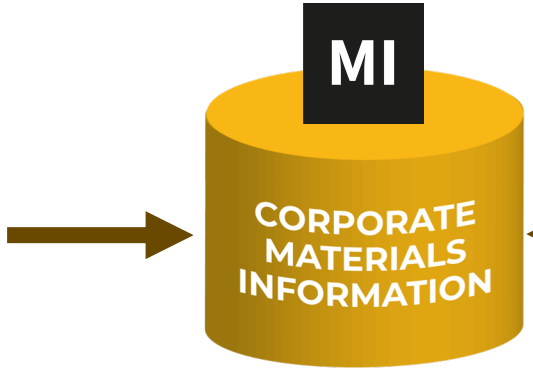
Example material data sets

GRANTA MI – ‘gold source’ for corporate material intelligence

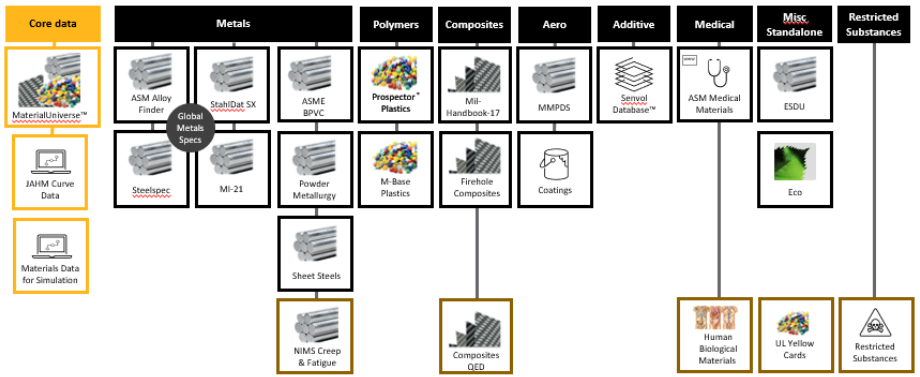
Aesthetic / Rendering	Basic material properties	Supplier specs
Detailed engineering properties	CAE models	Testing and analysis
In-service data	Compliance data	



Proprietary materials information



GRANTA MI

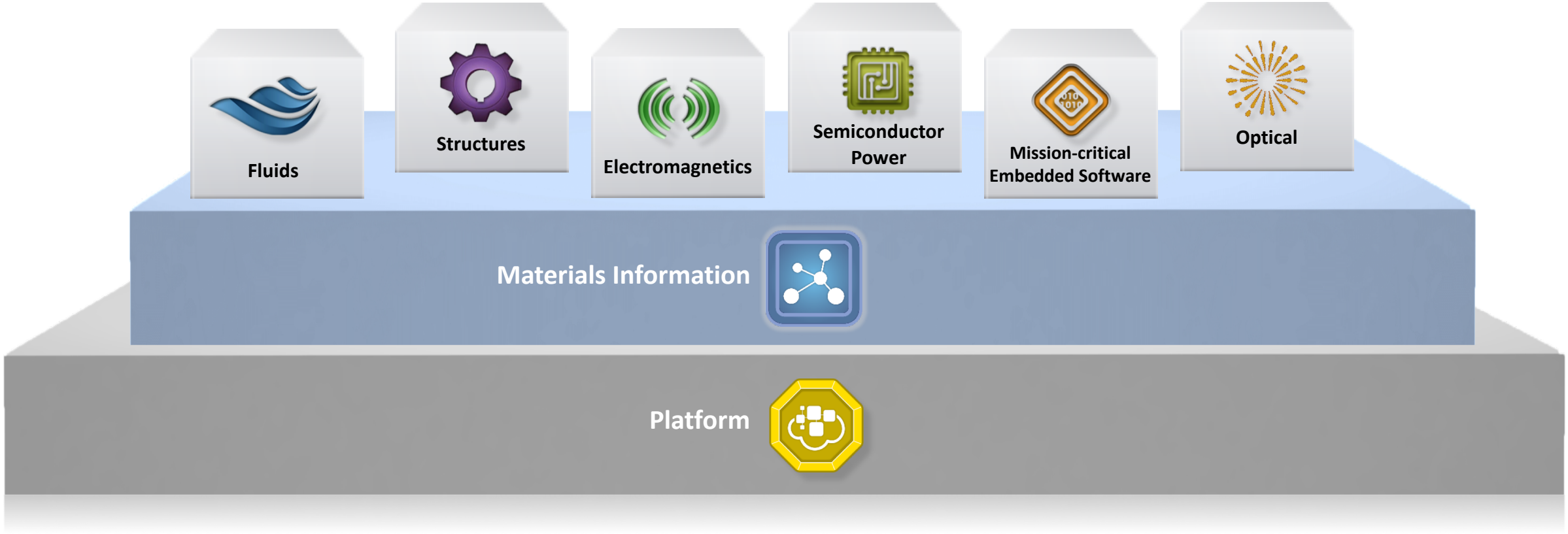


A comprehensive library of material reference information: Metals, plastics, composites…

Critical system requirements:

- Specialist materials data structures
- Tools to manage the materials data lifecycle
- Full traceability
- Access and change control, workflow

Ansys Granta: Materials Information for all Physics

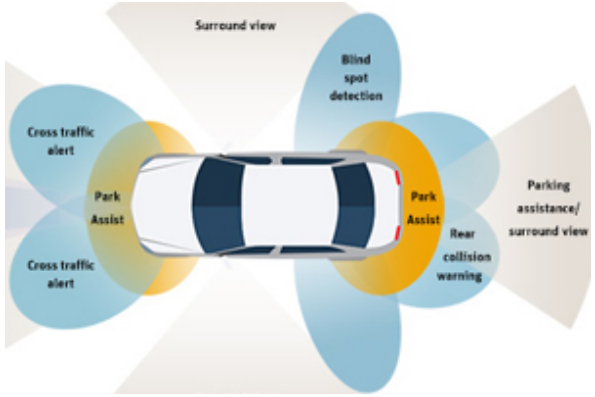


Materials challenges in EM design

Automotive Radar

Used for safety, navigation and driver assistance

- Antenna and sensors in close proximity to structure & bodywork
- Need to control scattering of beam
- Need *dielectric properties* of *automotive materials* at 24 & 76 GHz



High Speed PCBs

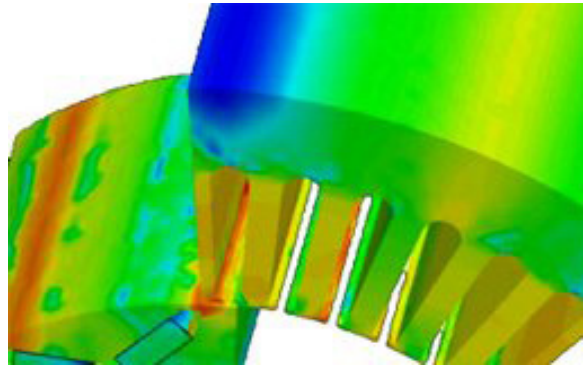
5G networks increasing data rates and frequency of PCBs

- Materials start to influence performance: PCB materials, effects of weave in PCB, surface roughness of copper
- SI simulation needs *dielectric properties* of *PCB* and *packaging materials* over a wide frequency range and which meet causality requirements

Electric Motor Design

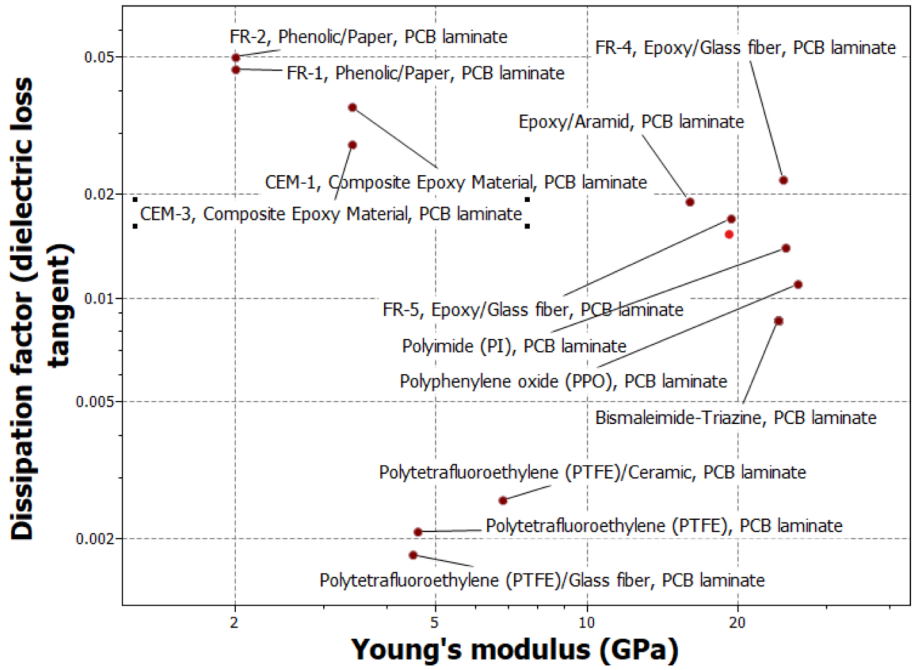
Automotive require lightweight, compact and quiet motors

- Coupled EM, mechanical and thermal analysis need multi-physics approach to materials
- *Magnetic*, *Mechanical* and *Thermal* properties required, all at elevated temperatures

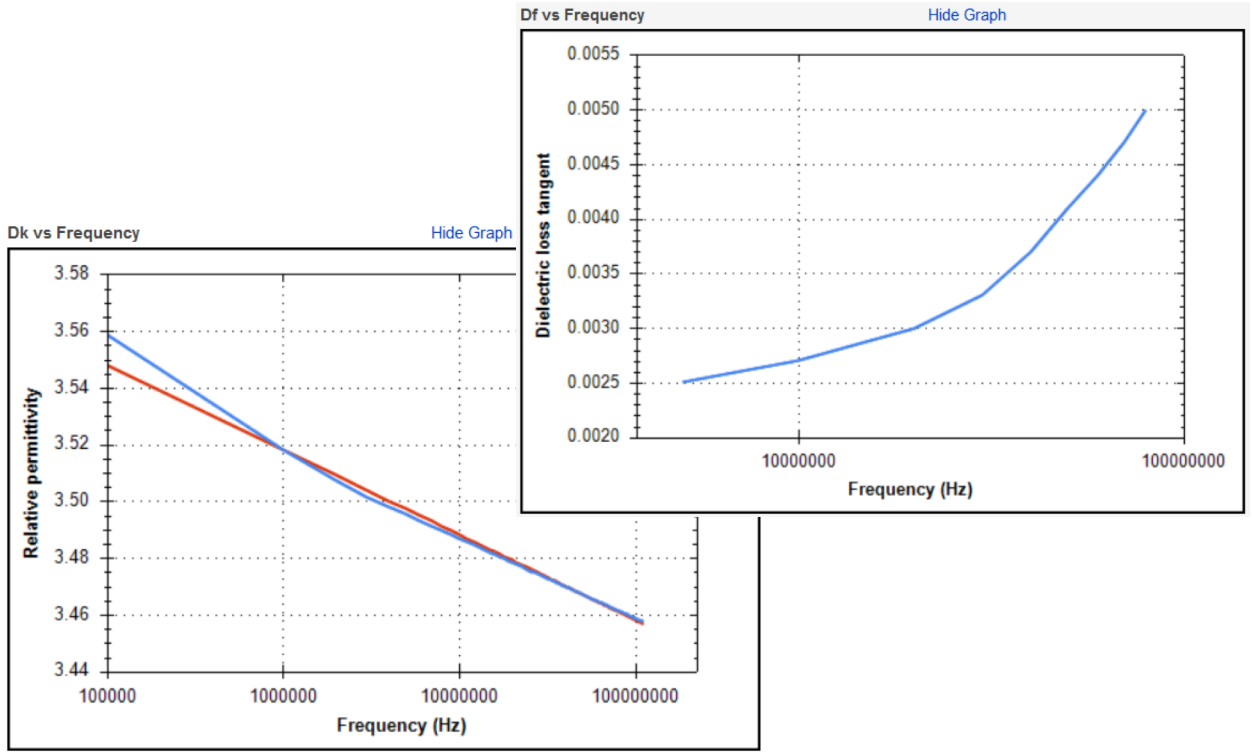


Importance of accurate materials properties: PCB Laminates

- Variation with material grade
  - Resin & resin content
  - Reinforcement type and style
  - Thickness of laminate and copper
  - Surface roughness

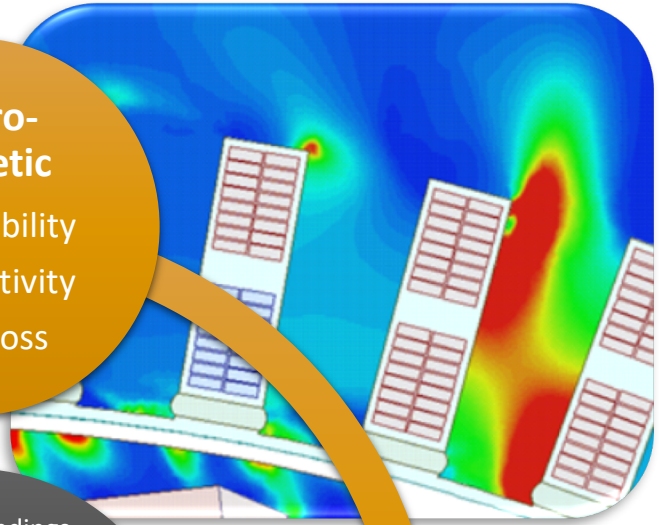


- Variation with operating condition



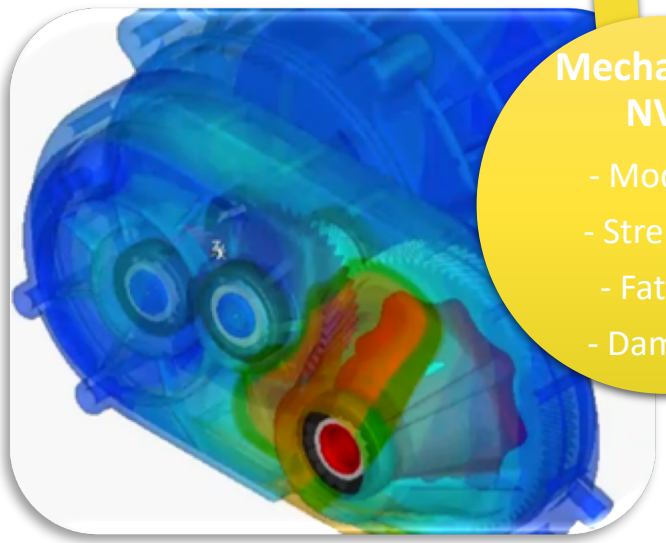
Multiphysics

Materials form a common link between multiphysics simulations



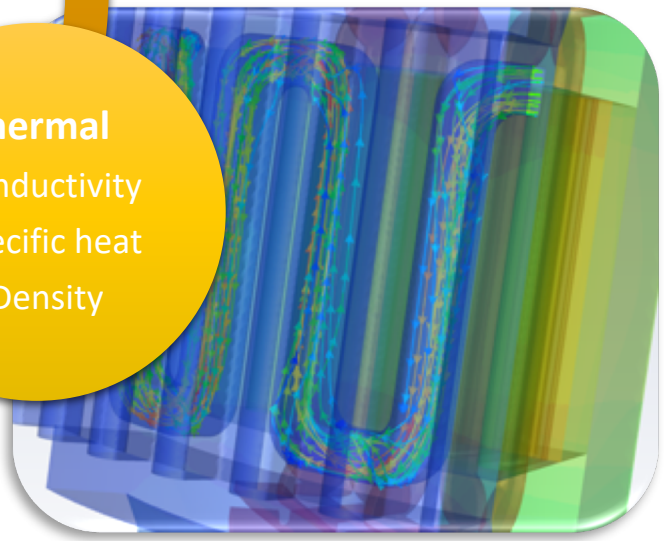
Electro-magnetic
- Permeability
- Conductivity
- Core loss

Copper windings
Hard magnets
Electrical steel laminates
Carbon brushes
Epoxy insulation
Cooling fluids
Nylon bearings
Steel casing

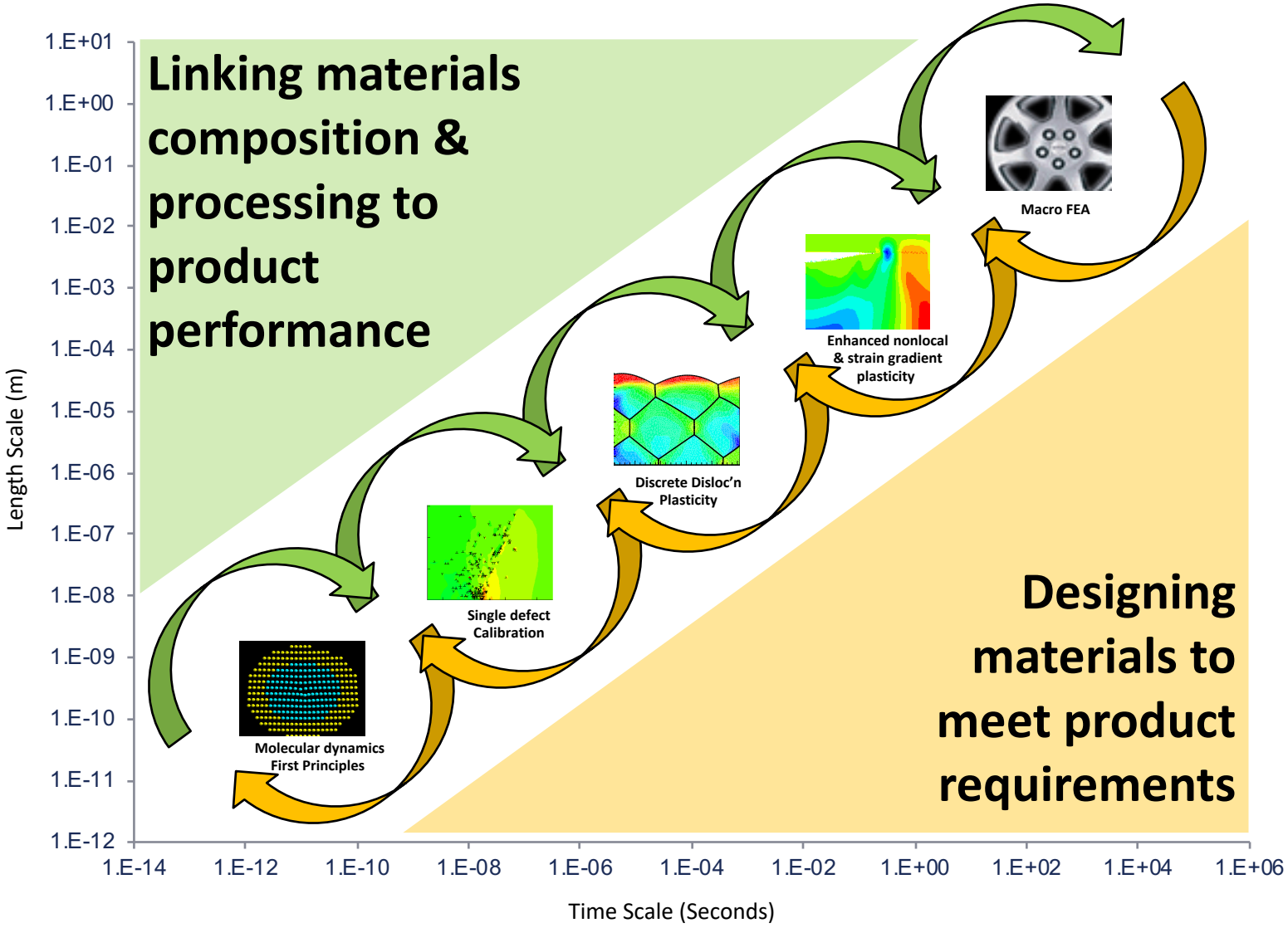


Mechanical/ NVH
- Modulus
- Strengths
- Fatigue
- Damping

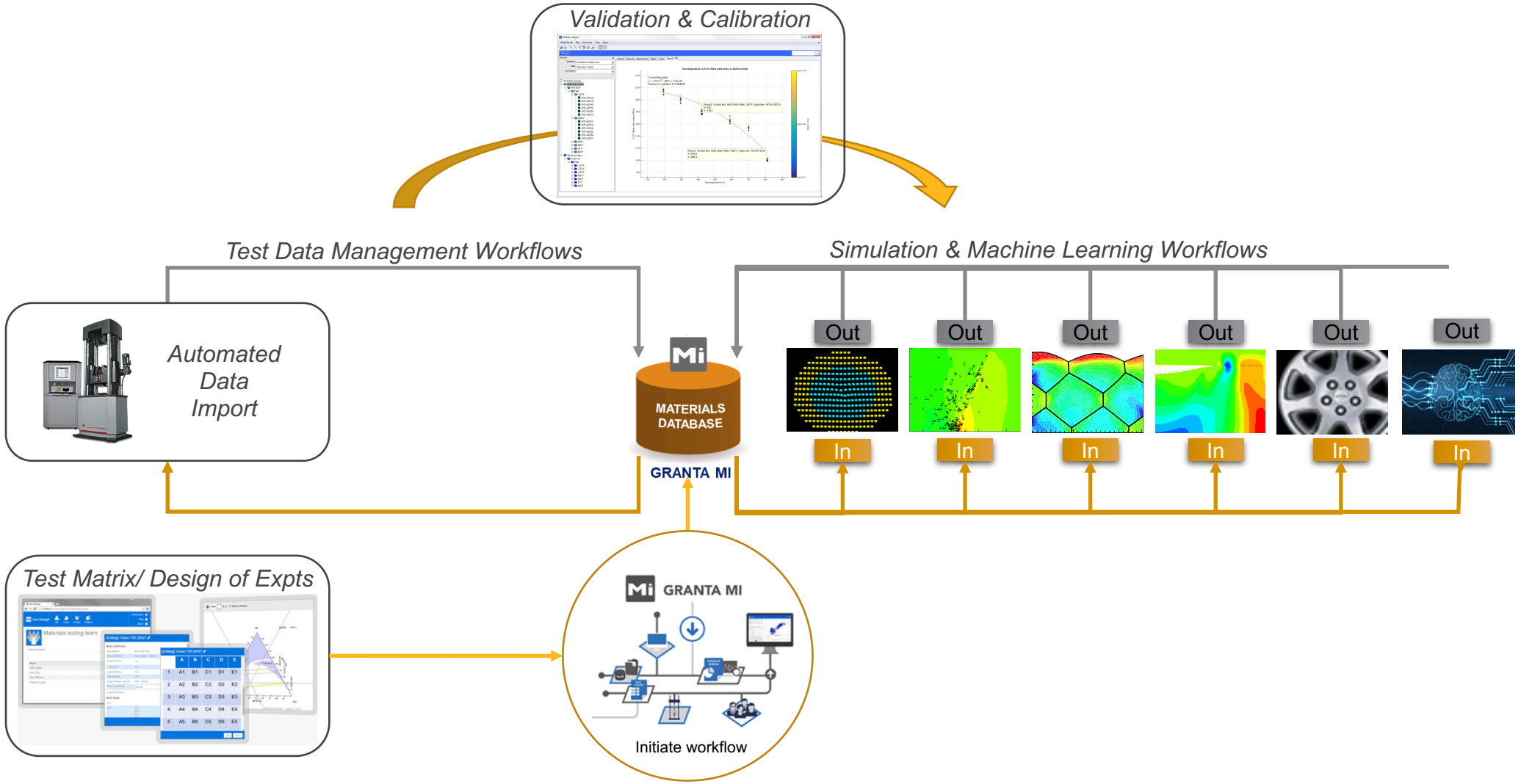
Thermal
- Conductivity
- Specific heat
- Density



Multiscale modelling



ICME: Integrated Computational Materials Engineering



Case Study: Materials Data for Organic Electronics

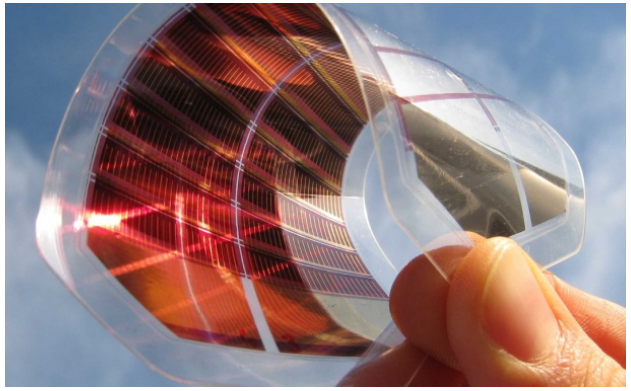
CORNET Project

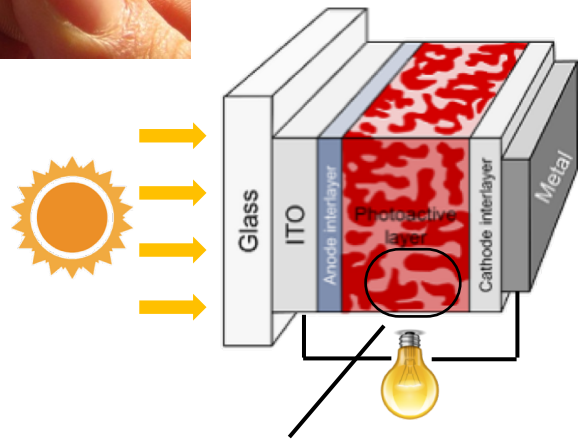
Ansys

CORNET Project

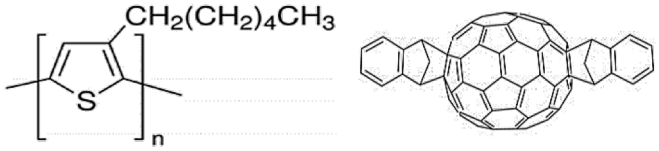
- CORNET Project : Multiscale Modelling and Characterization to Optimize the Manufacturing Processes of Organic Electronics Materials and Devices
- It is a 3 years research project funded by European Union under Horizon 2020 funding scheme (DT-NMBP-07-2017 call)
- It covers the triangle of manufacturing, modelling and experimentation to optimize the OPVs, PPVs, OLEDs
- It aims to develop a data management system for Organic Electronics (OE) materials information accommodating manufacturing process parameters, test and simulation data and agreed metadata
- https://www.cornet-project.eu/

CORNET: Organic electronic industry challenges





Photoactive layer:
Amorphous Donor-Acceptor blend



Organic Photovoltaics (OPVs)

- Light weight, flexible, low cost, printable
- Environmentally friendly
- Easy installation, ideal for complex surfaces

But…

- Low Power Conversion Efficiencies (<15%)
- Poor lifetimes (~1yr)
- Low carrier mobilities (10^{-6}-10^{-2}cm^2/Vs)

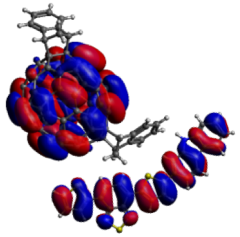
OPV Performance: strongly depends on materials used and processing conditions

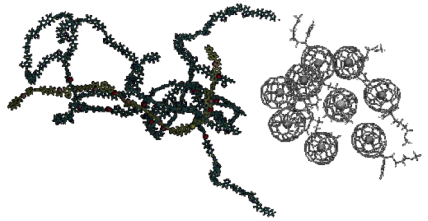
Non-Global, Non-Well-defined materials and process models as in Si-based PVs

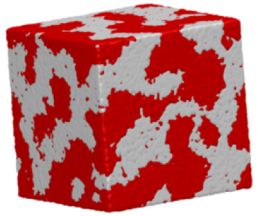
CORNET: Multiscale Modelling of OE materials

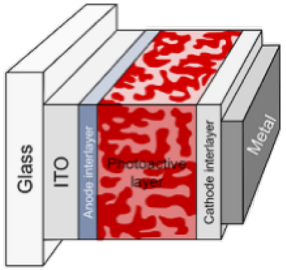
from electrons… **… to full device characterization**

electronic	atomistic	mesoscale	macroscale
Schrodinger equation for electrons	equations of motion for atoms & molecules	domains & stochastic charge transport	Drift-diffusion for carriers



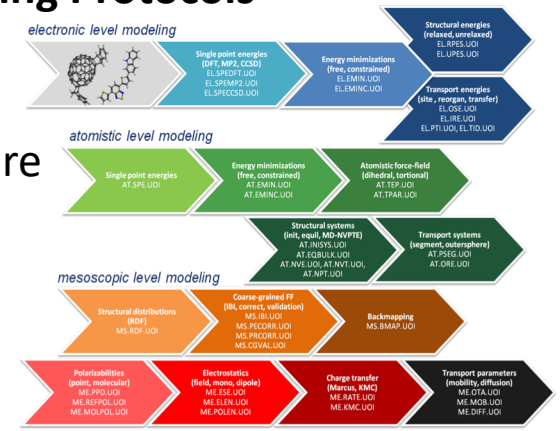






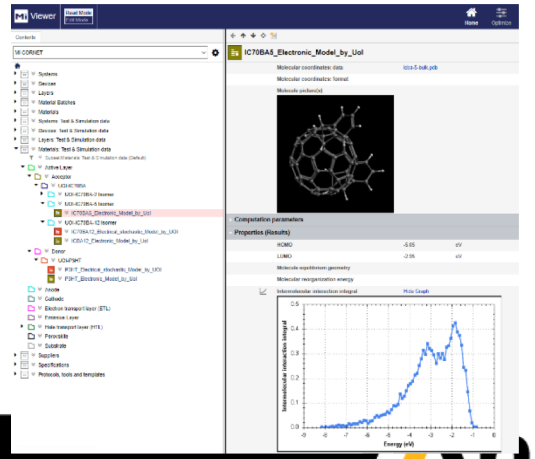
Modelling Protocols

- Physics
- Approximations
- Numerical procedure



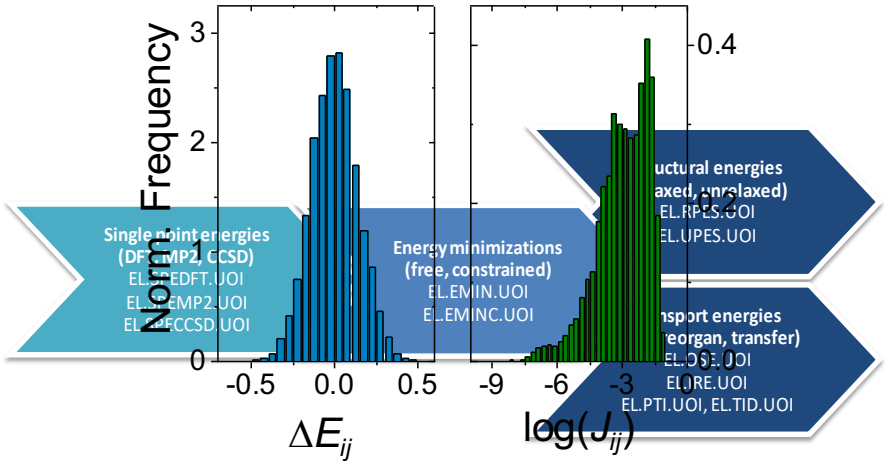
Data Management

- Data analysis tools
- Visualization
- Post-Processing

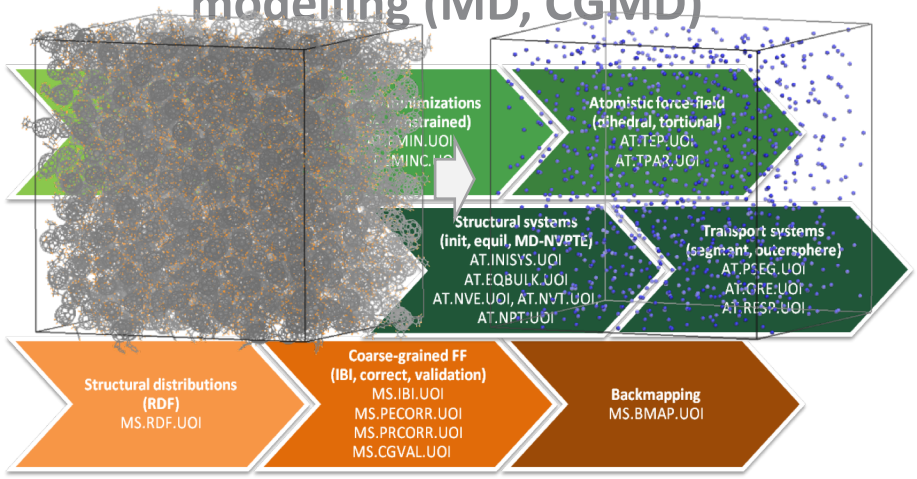


CORNET: Multiscale Modelling Protocols for OEs

Electronic modelling (DFT)



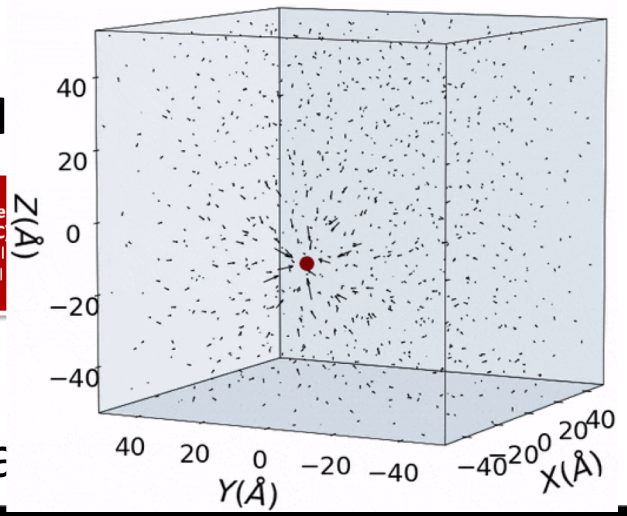
Atomistic & Mesoscopic structural modelling (MD, CGMD)



Charge transport within Marcus theory

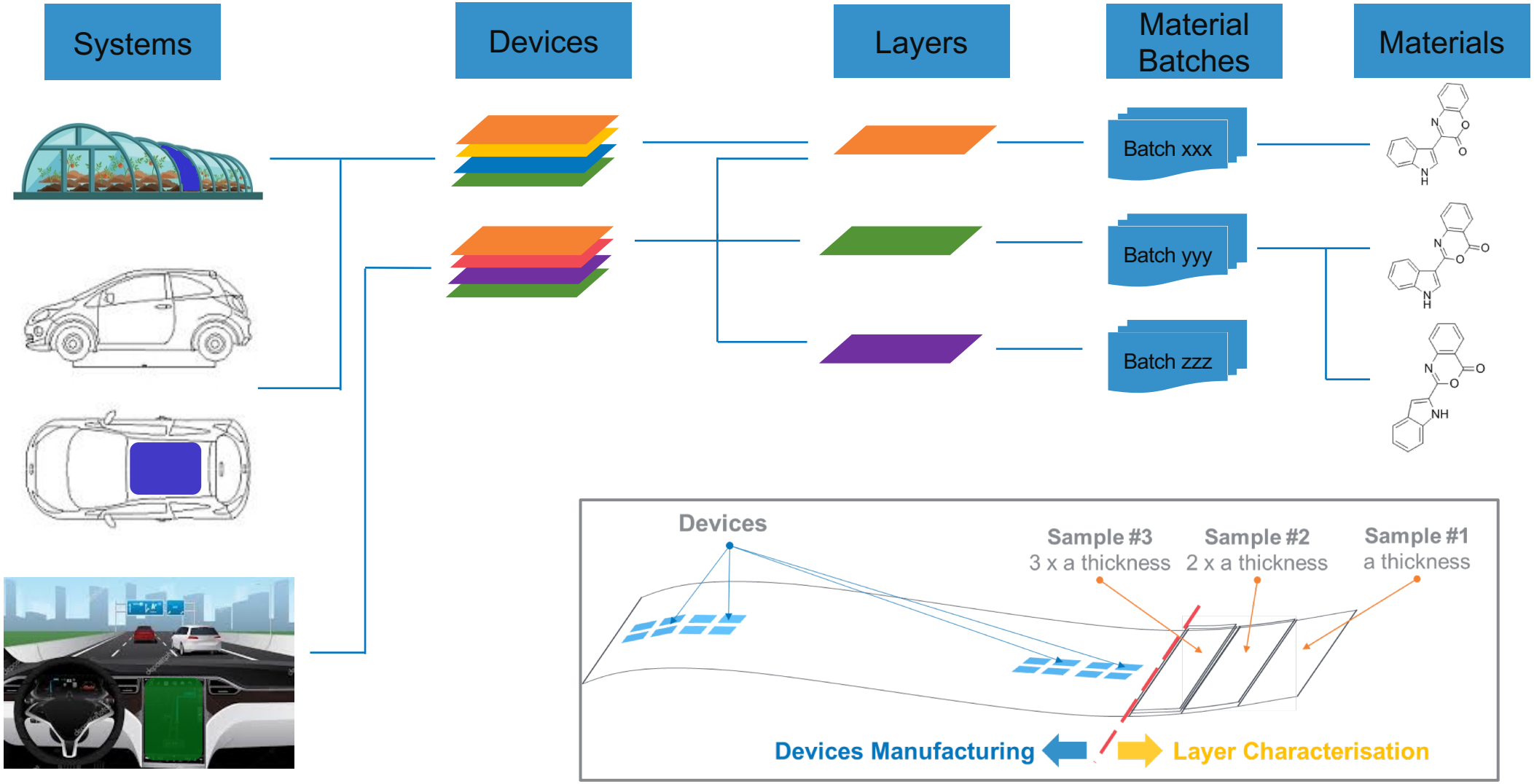
Mesoscopic electrical model

$$W_{ij} = \frac{2\pi}{\hbar} \frac{|J_{ij}|^2}{\sqrt{4\pi\lambda_{ij}k_BT}} \exp\left[-\frac{(\Delta E_{ij} + \lambda_{ij})^2}{4\lambda_{ij}k_BT}\right]$$

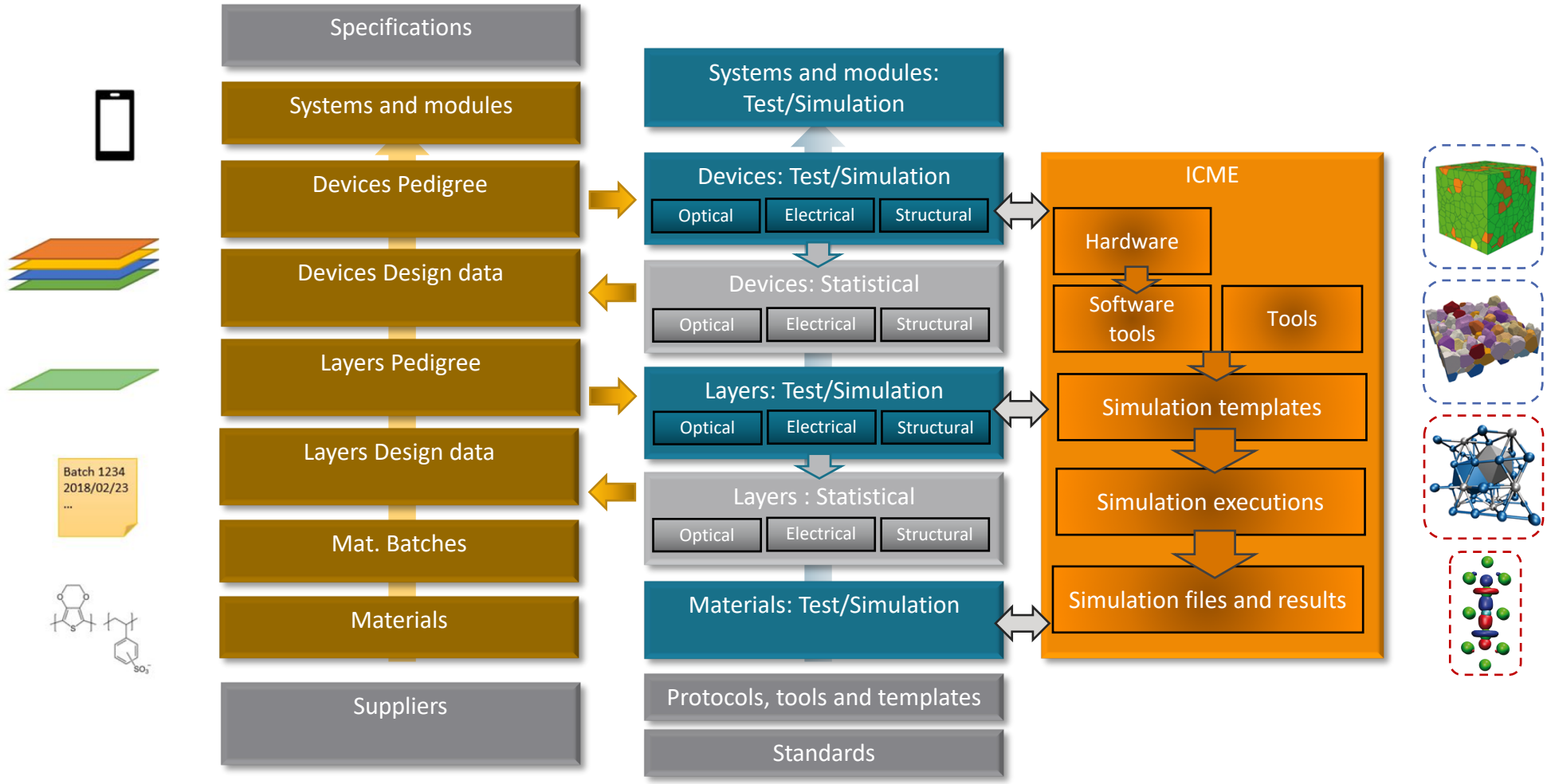


Protocol Chains spanning all length a

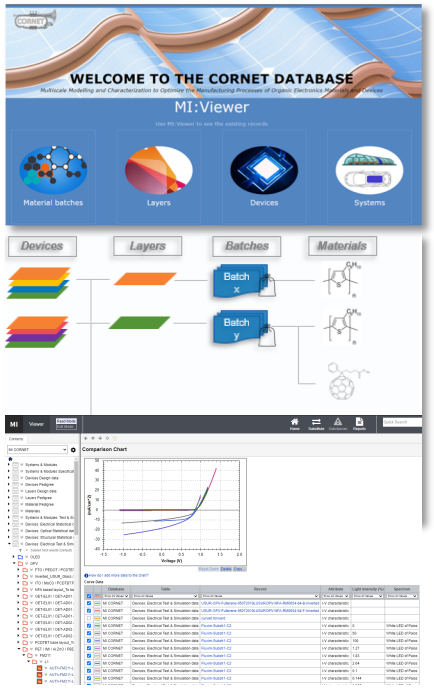
CORNET: Characterisation of Multilayer Devices



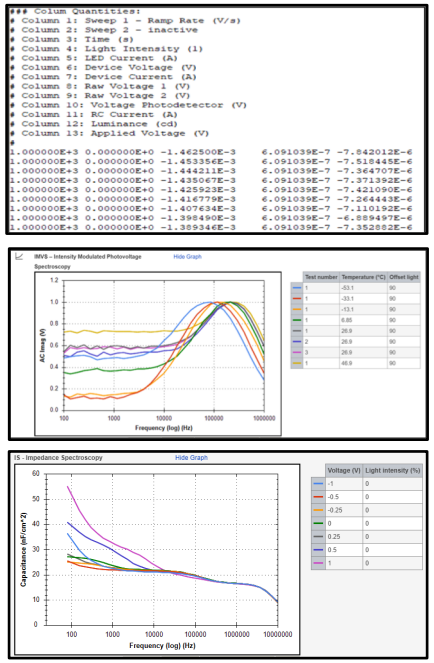
CORNET: Materials Data Management Structure



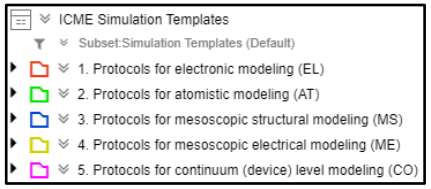
CORNET: Summary of Developments

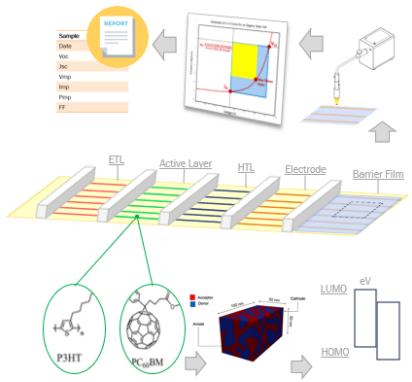


Data management for OE based on GRANTA MI technology



Capture of physical test data from electrical, structural and optical characterisation of OE devices, layers and materials





Collection of multi-scale materials modelling results and facilitation of model validation against physical test data

Digitalisation of characterisation and model validation protocols and capture of agreed metadata

CORNET: Acknowledgements & Contacts

University of Ioannina:

- Prof. Eleftherios Lidorikis, CORNET PI
  - elidorik@uoi.gr
  - +302651007146
- Prof. Dimitrios Papageorgiou
  - dpapageo@uoi.gr
- K. Kaklamanis, M. Andrea, K. Kordos, P. Palomino

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- Dr. Donna Dykeman, Programme Manager, Collaborative R&D
  - Donna.Dykeman@ansys.com
  - +44(0)1223218000

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