IM2D: an industry-driven interoperable solution for the simulation-aided design of emerging electronics

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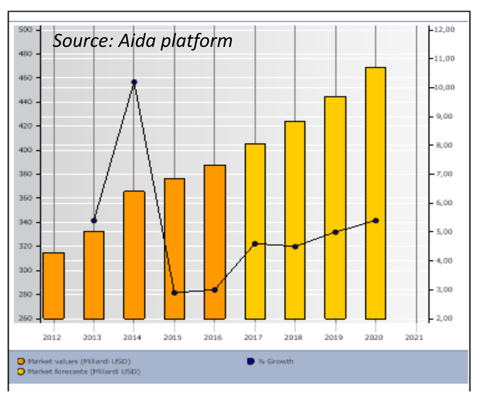
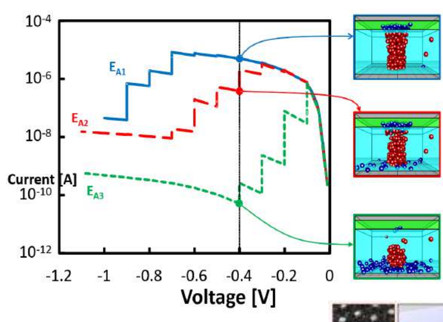
Motivations and background

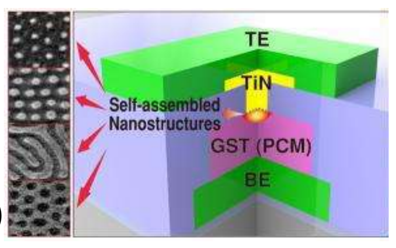
The *new wave* semiconductor industry

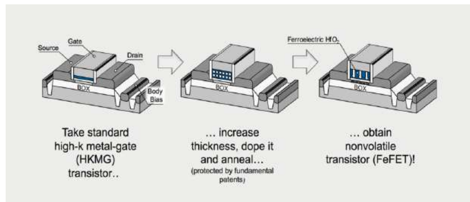
- The world value of the **semiconductor market** is approx. € 423 billion
- Currently, **Europe** is at current 9% world share. Europe's **ambition** is to attain 20% world market share in the semiconductor industry.



- Semiconductor industry and electronics are in an **expansion** stage
- Semiconductor leaders are taking a future-oriented approach and considering new end **markets beyond the PC**, such as AI, IoT, and autonomous vehicles.







Memory devices or storage-class memories

Challenges and open problems
- complex non-Si-based materials (chalcogenides, metal-oxides, ferroelectrics, etc)
- high-defects, disorder and amorphous
- complex physical effects (electrical switching, quantum confinement, topology, spin, etc)
- device reliability & variability
- complex architectures

Priories for new electronics
- characterization/optimization/design of materials

&

- characterization/ optimization/ design of devices

Materials at device level

- The **interplay** between **materials** and the influence they have on the **device** is hard to determine.

Need for investigation of materials at device level: the materials characteristics are inherently connected to the device performance requirements

Industry needs

Tremendous challenge for industrial users → **huge amount** of
- time
- material and personnel consumption
- advanced technical skills
- data analysis

→ **High costs**

Modelling

Can efficiently contribute to industrial innovation
- reduction of experimental trials
- new top-down and bottom-up design paradigms
- understanding of physical mechanisms
- robust and validated results

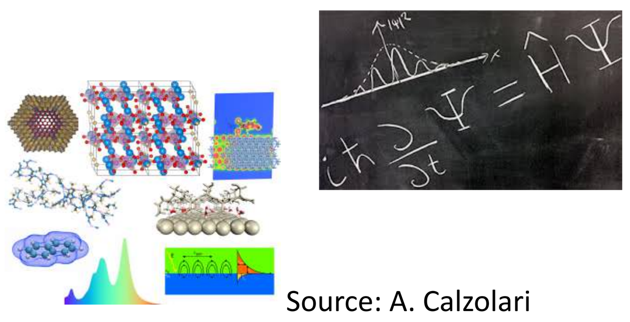
→ **Reduction of costs and time to market**

Concept & Interoperability

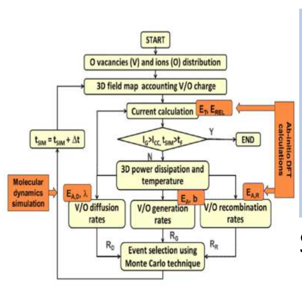
Electronic and atomistic software

- mature reality for high-level materials modelling
- scientifically driven but not industry driven
- requirement of advanced specialized skills

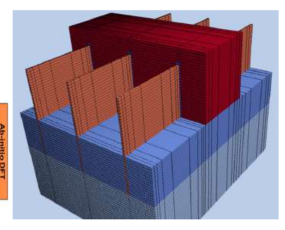
Such know-how is thus **not readily available to industry**, especially in SMEs that often lack R&D resources



Source: A. Calzolari



A. Padovani et al. IEEE TRANS. ELEC. DEVICES, VOL. 62, NO. 6, JUNE 2015



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Industry-driven software

- optimized to model complex devices and circuit architectures,
- based on characteristics of the material in the device configuration

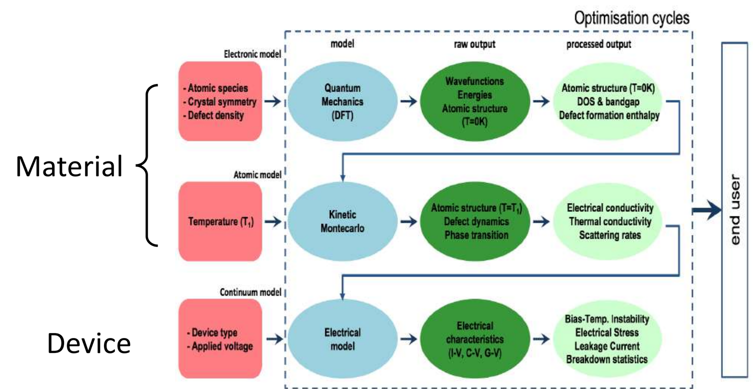
These parameters are **not available for complex materials**, such those used for synaptic electronics

At present materials and device modelling are far apart

OUR STRATEGY
re-use and **integration** of existing software and interoperability are key to provide **industry-ready software solutions** that can be taken by third parties

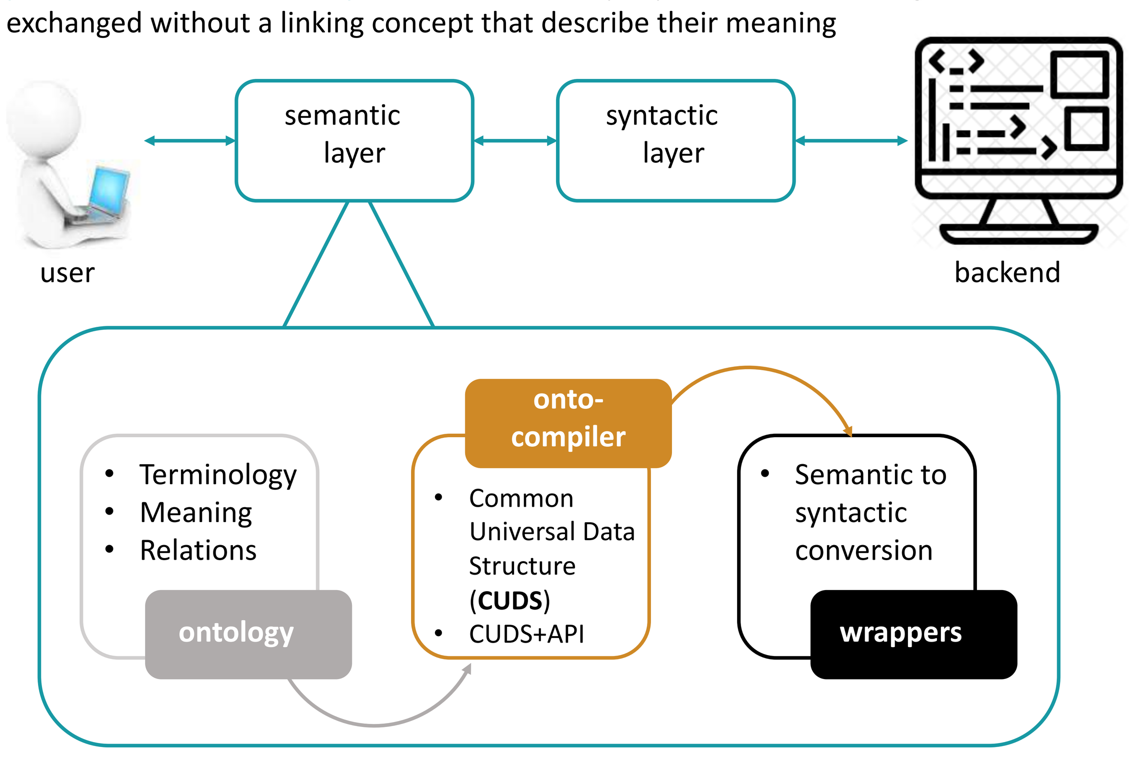
Ontology-based Interoperability

- Level I: syntactic interoperability → structural interconnections among physical models and codes, e.g. **coupling-and-linking** of models and the generation of a **data pipeline** between existing codes

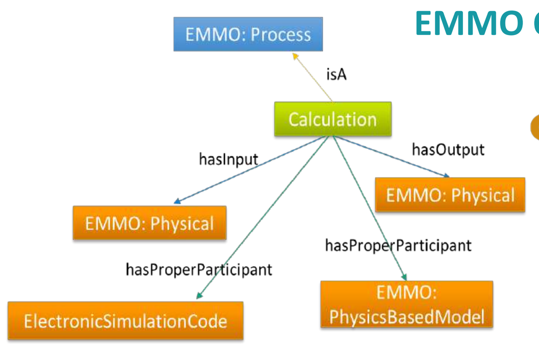


- **Necessary** for automation, data curation and traceability
- **Not sufficient** to reduce the complexity of the problem → need to go beyond software compatibility
- Formalize and implement **workflows specific to target users' needs and skills**

- Level II: semantic interoperability → the description of the information **meaning** in a formal and machine-readable and **processable** way (metadata and schema based on semantics) → interdependence between concepts and data: concepts provide the meaning for a set of data ←→ data sets cannot be exchanged without a linking concept that describe their meaning



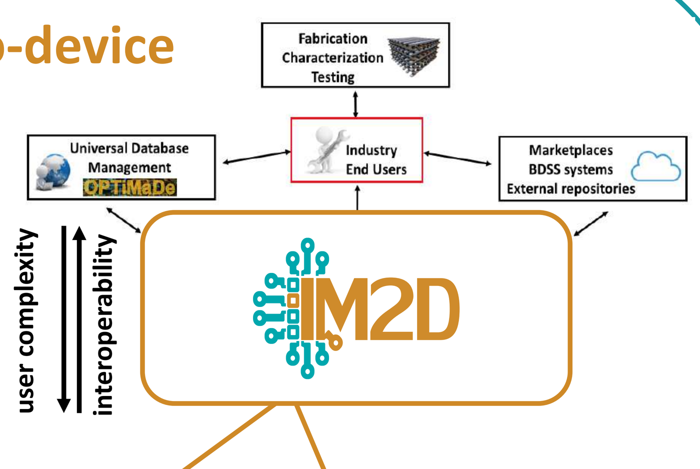
EMMO Ontology extension to electronics domain

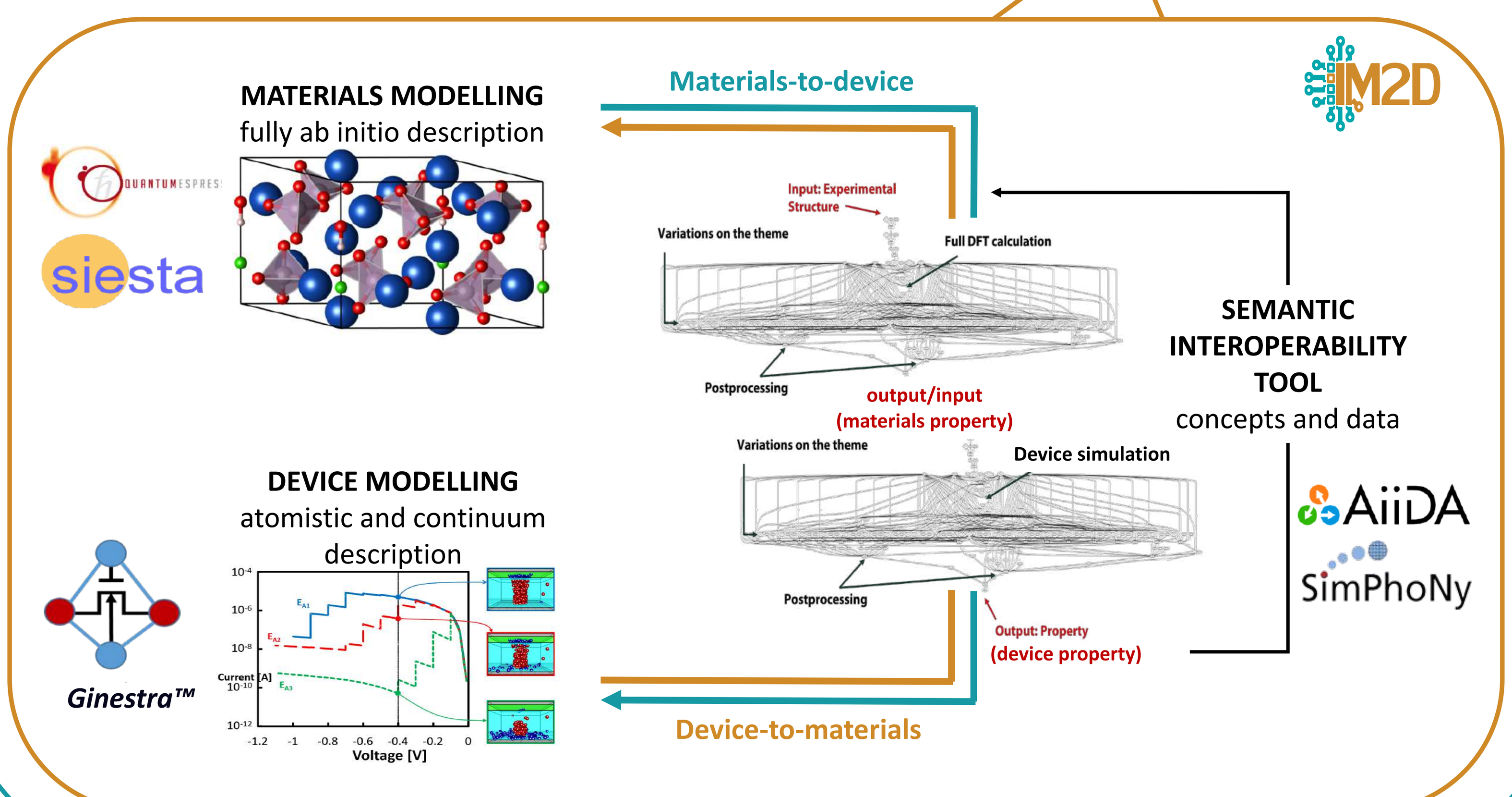


- Formal standardization of
  - **physical quantities** (materials entities, models, materials relations)
  - **calculation type**

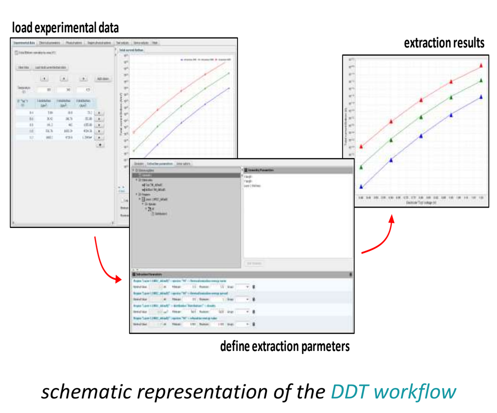
IM2D - interoperable materials-to-device

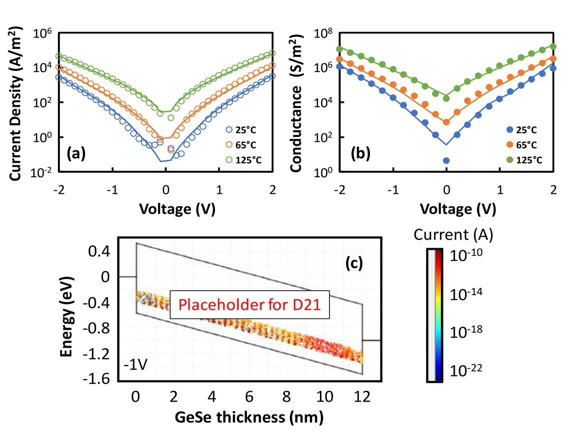
IM2D → multi-physics, multi-model, multi-equation, hierarchical and scale-reversible model for material-to-device and device-to-material optimization for an easier exploration of the material workspace **from** an electronic **device-oriented industrial perspective**

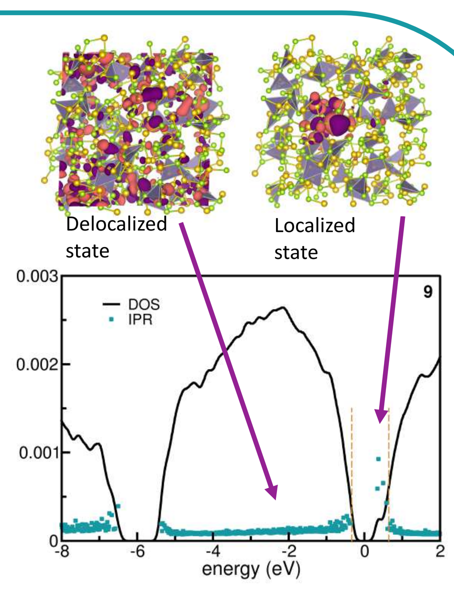




Traps in TiN-$Ge_{50}Se_{50}$-TiN MIM selectors







Device-to-materials workflow
- Measured experimental data are loaded into the *defect discovery tool* of Ginestra™ (DDT) the gate leakage currents as a function of the temperature.
- Device, material and trap parameters to be extracted (as well as their variation ranges) are selected from a dedicated panel of the DDT.
- Comparison/analysis with DFT simulations.

MIM electrical characterization (IMEC)
(a) Current and (b) conductance densities simulated (lines) and measured (symbols) at different temperatures on 20nm-thick TiN/$Ge_{50}Se_{50}$/TiN capacitors.

DDT MIM defect analysis (AMAT)
The defect bands extracted from the DDT fitting D21 I-V and G-V data are located on average at ~0.45eV from $Ge_{50}Se_{50}$ valence band top.
→ Effective Se vacancies (deficiencies)

DFT materials analysis (CNR)
- Model structure for amorphous structure at room temperature → local-order and folding structures
- Average model has a mobility gap of ~1.0 eV partially filled by localized states (traps)
- Trap states localized on low-coordinated Ge-structures and Ge-Ge chains → effective Se-vacancy defects

Funding

INTERSECT - interoperable material-to-device simulation box for disruptive electronics

A H2020-NMBP-TO-IND-2018 funded project: GA n. 814487

Links

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